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MODELLING LEAD IN DRINKING WATER

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SUMMARY

In light of substantial medical evidence of the detrimental effect of lead on the body, the use of lead in pipe networks, and the subsequent lead emissions into drinking water is now a major concern. As a result, the new European Union "drinking water" directive requires the standard for lead in drinking water to be tightened from 50μg/l to 25μg/l by December 2003 and to 10μg/l by December 2013.

It is anticipated that these standards will be achieved by a combination of water treatment, which must be optimised, and selective lead pipe replacement where necessary. In order to optimise corrective treatment, accurate monitoring of lead emissions across a water supply zone must be achieved. The severe limitations of traditional monitoring methods have provided the motivation to develop a computational model to facilitate the optimisation of corrective treatment as well as to investigate lead emissions at individual houses.

The development of a model to assess lead emissions in drinking water at a single house and across a water supply zone is described. The model has been used to investigate the daily variation of lead emissions at a single house and to determine the influence of factors, such as pipework geometry and water usage, on the daily average concentration of lead in drinking water. The ability to simulate traditional sampling methodologies on simulated water supply zones has enabled the model to be validated for a wide range of real water supply zones. This has allowed the model to be used successfully for the purposes of assessing zonal compliance and facilitating the optimisation of corrective treatment. Additionally, the model has enabled a detailed assessment of the use of the Random Day Time sampling method, for the optimisation of plumbosolvency control.

DECLARATION

This work has not previously been accepted in substance for any degree and is not concurrently submitted in candidature for any degree.

Signed .... (candidate)

Date 29/05/2004

STATEMENT 1

This thesis is the result of my own work/investigation except where otherwise stated. Other sources have been acknowledged by footnotes giving explicit references. A bibliography is appended.

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I hereby give consent for my thesis, if accepted, to be available for photocopying and for inter-library loans, and for the title and summary to be made available to outside organisations.

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CONTENTS

FIGURES AND TABLES

NOTATION

$\bar{c}$	($\mu g/l$)	Mean concentration during flow (volume-weighted)
$\overline{F}$	-	Mean number of samples that fail
θ	-	Angular coordinate axis
ρ	(kg/m^3)	Density
μ	(kg/ms)	Viscosity (dynamic)
μ	-	Mean
σ	-	Standard deviation
Δx	(m)	Increment in x-direction
$30MS$	($\mu g/l$)	30 Minute Stagnation Test sample concentration
A	(m^2)	Area (pipe cross-section)
a_j	(m^2)	Area (cross-sectional) of annuli j
A_s	(m^2)	Internal surface area
c	($\mu g/l$)	Concentration of lead in water
c_0	($\mu g/l$)	Initial concentration
$c_{average}$	($\mu g/l$)	Mean concentration during stagnation (area-weighted)
C_T	-	Number of shared communication pipes in zone
D	(m^2/s)	Diffusion coefficient
D	(m)	Diameter
DAC	($\mu g/l$)	Daily Average Concentration
D_{Cu}	(m)	Diameter of copper pipework
D_F	(m_2/s)	Diffusion coefficient (during flow)
D_{Pb}	(m)	Diameter of lead pipework
E	($\mu g/l$)	Equilibrium concentration of lead in water
F	-	Number of samples in a RDT survey that fail
$f(r)$	($\mu g/l$)	Initial concentration distribution across cross-section of pipe
F_k	(s)	Flow time for kth time period
F^T	(s)	Total flow time in one day
g	(m/s^2)	Gravitational acceleration
H_0	-	Null Hypothesis
H_1	-	Alternate Hypothesis
H_T	-	Number of houses in zone
i	-	Element position in x-direction
Int	-	Integral
j	-	Element position in r-direction
J	-	Number of elements in r-direction
J_0	-	Bessel function of the first kind of order zero
J_1	-	Bessel function of the first kind of order one
k	-	Time period
L	(m)	Length of pipe

L_{Cu}	(m)	Length of copper pipework
L_{Pb}	(m)	Length of lead pipework
m	-	Number of simulated sampling surveys
M	$(\mu g/m^2/s)$	Initial mass transfer rate
M_∞	(μg)	Quantity of lead generated in time ∞
M_t	(μg)	Quantity of lead generated in time t
n	-	Number of timesteps
n	-	Number of Bessel roots
N	-	Number of elements in x-direction
p	(N/m^2)	Pressure
P	-	Number of time periods in one day
P	-	Probability (statistical significance)
$Pb\%$	$(\%)$	Proportion of houses supplied through lead pipework
P_k	$(\%)$	Proportion of total volume of water for kth time period
Q	(m^3/s)	Volumetric flow rate
r	-	Radial coordinate axis
r_0	(m)	Radius (internal)
Re	-	Reynolds number
s	$(\mu g/l)$	Testing limit
S	$(\mu g/s)$	Generation of lead
S_k	(s)	Stagnation time for kth time period
t	(s)	Time
T	(s)	Total time of flow/stagnation
u	(m/s)	Velocity of fluid in x-direction
U	-	U-Statistic
$\bar{u}$	(m/s)	Mean velocity in x-direction
u_{max}	(m/s)	Maximum velocity in x-direction
v	(m/s)	Velocity of fluid in r-direction
V	(m^3)	Volume
V^T	(m^3)	Total volume of water used in one day
w	(m/s)	Velocity of fluid in θ-direction
x	-	Longitudinal coordinate axis
Y	(s)	Length of each time period
Z	-	Standard Normal Deviate
α_n	-	Roots of Bessel function
Δr	(m)	Increment in r-direction
Δt	(s)	Increment in time, i.e. timestep
λ	-	Friction factor
τ	(N/m^2)	Shear stress

PREFACE

This thesis is broken into four main chapters. The first chapter 'The Problem' establishes the motivation and sets the objectives of the research as well as outlining various aspects of the problem. Lead poisoning, in particular relation to drinking water, is described. Regulatory issues, including water quality regulations, strategies for corrective action and compliance assessment methods are discussed. In particular, limitations of existing compliance assessment methods are examined, providing the motivation for the research. Chemistry of lead in drinking water is briefly described, with particular emphasis on solubility of lead in drinking water and the concentration versus time relationship. Additionally, the factors that are thought to affect lead emissions in drinking water at a single house as well as across a water supply zone are discussed.

The second chapter 'Single House' describes the development of a model to predict lead emissions at a single house and its subsequent employment for investigating the influence of household parameters on lead emissions. This includes a description of the mathematics that describes the underlying physical processes that influence lead emissions at a single house, such as flow and mass transfer. The development of the model is then described in terms of the assumptions that are required to represent the influencing characteristics at a house as closely as possible and the application of the mathematics previously described. Results, in terms of the variation of lead emissions over time, for a single house are presented. This is followed by an in depth sensitivity analysis intended to determine the influence of each parameter, e.g. daily water consumption, on lead emissions. Experimental work carried out to determine the solubility characteristics of various different waters is described.

The third chapter 'Water Supply Zones' describes the development of a model to predict lead emissions across a complete water supply zone and its subsequent employment for predicting compliance with the water quality standards. This includes a description of the mathematics that describes the parameters that effect lead emissions within zone. The development of the model is then described in terms of the assumptions that are required to represent the influencing characteristics of a zone as closely as possible as well as the approach for simulating various compliance assessment methodologies. Results for the variation of lead emissions across a zone and the simulation of various compliance assessment methodologies is presented. This is followed by an in depth sensitivity analysis intended to determine the influence of each zonal parameter on compliance assessment results. The extension of this model to zones having shared communication pipes is discussed and the influence of shared communication pipes is investigated.

The fourth chapter 'Using the Models' describes how the models have been employed to assess the compliance of real water supply zones and to facilitate the optimisation of corrective treatment. Validation of model results for a wide range of real water supply zones in demonstrated. A real world example of the employment of the model for investigating the likely effects of corrective water treatment and selective lead pipe replacement is discussed; in particular, the optimisation of corrective water treatment is demonstrated. A real world example relating to a zone having shared communication pipes is

described. Finally, the suitability of the random daytime sampling method of compliance assessment, for the purposes of optimisation of corrective water treatment, is investigated using the model.

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I have been lucky enough to carry out my PhD in the Department of Civil Engineering at the University of Wales, Swansea, which has an outstanding worldwide reputation for research and includes staff members that are internationally leading experts in their field. However, I will remember the Department most for the friendliness and kindness that both teaching and administration staff have shown, which has made me feel at home from the very beginning.

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Daniel Van der Leer
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1 THE PROBLEM

1.1 Background and motivation

1.1.1 Lead

Lead (Pb) is a silvery-white or bluish-grey metal in Group IVa of the periodic table, which occurs naturally in the earth's crust. Lead rarely occurs in the elemental state, however, it is found in a number of ores, in particular lead sulphide, otherwise known as galena (PbS). Lead ore is mined and the lead can be smelted (extracted) from the ore by a roasting process - that is, convert it to the oxide, and reduce the oxide with coke in a blast furnace. Lead has been mined and smelted for at least 8,000 years. This has been confirmed by artefacts in various museums and by ancient histories and other writings, including the biblical Book of Exodus. [1] Known in antiquity and believed by the alchemists to be the oldest of metals, it was associated with the planet Saturn.

For a metal, it is dense at 11.34 tonnes/m^3 (at 20° C) and has a low melting point of 327.4° C. Lead is also very soft, highly malleable, ductile, and is a poor conductor of electricity. It is easily formed, cut and jointed and its flexibility provided resistance to subsidence and frost. It has also been found to be highly durable and resistant to corrosion. These useful properties set it apart from other metals, facilitating its widespread application, by humankind, throughout history.

Lead was used prolifically by the ancient Romans, where it was deemed suitable for a vast variety of everyday uses. These included everything from its use as a seasoning and preservative in foods and drinks to its use as a material to make pots, pans and pitchers from, due to its abundance and malleability. Indeed, leads remarkably useful properties, including its resistance to fracture, made it ideal as a piping material for the vast network plumbing that kept Rome and the provincial cities of the Roman Empire supplied with water. Lead has also been used throughout history as a pigment in paints, and in the case of the ancient Egyptians, a key component in cosmetics such as face powders.

Despite leads toxic effects on human health, which will be outlined in the proceeding chapter, it has continued to be used in a wide range of products, applications, and processes, up to the present day. Until recently it has been used in many countries as the material of choice for water pipes in plumbing systems, due to its malleability and durability. Lead is also used in enormous quantities in storage batteries and in sheathing electric cables. Large quantities are used in industry for lining pipes, tanks, and X-ray apparatus. Because of its high density and nuclear properties, lead is used extensively as protective shielding for radioactive material. Among numerous alloys containing a high percentage of lead are solder, type metal, and various bearing metals. A considerable amount of lead is consumed in the form of its compounds, particularly in paints and pigments [2]. Lead has also been used extensively in petrol as a lubricant and to help reduce engine knocking.

1.1.2 Health aspects

Despite its numerous beneficial properties, described previously, lead is a highly toxic substance that does not have any useful biological function in humans or animals. Historically, however, it has been used as the primary ingredient for many traditional Eastern remedies. Rather ironically, these remedies were often used to alleviate or prevent the symptoms that they were actually likely to cause or enhance.

Lead is a cumulative poison, meaning that it builds up within parts of the body over many years of exposure, whether it is through ingestion of lead within food or drink, or through inhalation of lead within the atmosphere. Lead is readily absorbed through the gastrointestinal tract into the blood. After prolonged exposures a balance is achieved between that absorbed by soft tissues and that excreted in urine, faeces or sweat. Although body fluid and soft tissue equilibrate reasonably fast, reflecting current exposure to lead, bone and teeth have the ability to continue to accumulate lead with time thus reflecting long-term exposure [3]. The Romans were aware of some of the adverse health effects of lead, however, they carried on using it because they were so fond of its properties. They equated limited exposure to lead with limited risk, not realising that their everyday low-level exposure to the metal rendered them vulnerable to chronic lead poisoning, even while it spared them the full horrors of acute lead poisoning [4]. Indeed, it has often been suggested that this slow poisoning from lead is responsible for the decline of the Roman Empire.

Even at low levels, lead reacts with the enzymes, reducing their activity, within the body to slow or stop essential physiological reactions. [5]. Symptoms of low-level exposure, which often leads to chronic lead poisoning, include anaemia, anorexia, high blood pressure, abdominal pains, and in some cases mild neurological effects such as mood disturbances and loss of coordination. Symptoms associated with acute lead poisoning, particularly over long periods of time, include permanent damage to the kidneys, brain and nervous system. Lead affects many different areas of the brain including the cerebral cortex, cerebellum and hippocampus. The structure of blood vessels in the brain may also be altered, which can lead to bleeding and brain swelling [5].

The most sensitive target group, even for short-term exposure, are young children and pregnant woman. Growing children absorb lead more rapidly than adults do because of their body weight and metabolic differences [5]. Lead exposure in children has been associated with reduced IQ, learning disabilities, decreased growth, hyperactive and antisocial behaviour, and impaired hearing [6].

Numerous studies, which connect adverse health effects with exposure to lead, in humans, have been published. These date as far back as the beginning of the 19th century, an early example of which is a case published by Wolffhügel (1887) who stated that human disease could clearly be connected with the high lead concentrations found in the water of the German town of Dessau [7]. Studies carried out in the 1960s and early 1970s described cases of lead poisoning caused by prolonged ingestion of soft water containing excessively high levels of lead [8,9,10]. More recently, studies have revealed that there is a strong correlation between lead content of drinking water and blood lead levels [11,12,13,14,15].

1.1.3 Sources of lead intake

Lead naturally occurs widely throughout the environment and can often be found, in small quantities, in soils, plants, and waters. Consequently, ingestion of small quantities of lead is virtually unavoidable. The three primary sources of lead intake are through food, water, and air; however, different proportions of the lead intake are actually absorbed dependant on the source. It has been estimated that for intake through food, between 5 and 10% is absorbed, for intake through water, 10% is absorbed, and for intake through air, 35% is absorbed [3,16].

Industrial processes involving lead, and the mining of lead, have often caused elevated lead levels in soils and water through contamination, which, in turn, has caused high lead content in plants and crops. In this way, lead can be passed on through the food chain, affecting numerous species including humans. Even in the absence of any lead pollution or contamination it is very difficulty to produce food completely free of lead because of the abundance of lead in the environment. Foods most prone to elevated lead concentrations include dried foods, canned foods, liver, and vegetable that have a high area to mass ratio [17].

Lead levels within food and drink are sometimes elevated by the way they are stored or prepared. Although it is being phased out in some countries, lead solder is still widely used throughout the world to seal canned food; this can greatly elevate the lead content within the canned food, particularly if the food is acidic. High levels of lead have also been found in drinks such as cider, wine, and whiskey. Historically, lead has been used as a sweet and sour condiment, as well as a wine preservative; it should also be noted that one of the biggest sources of lead in the diet of the ill-fated Romans was from acidic food, fruit juices, and wines that were stored in lead-lined bronze utensils. Another source of lead ingestion is from the use of inadequately glazed ceramic vessels for food storage and cooking [17].

Lead is also present in drinking water wherever the water has been in contact with lead plumbing or lead based solders. Lead levels within water vary significantly and are dependant on numerous factors including water-lead contact time, water chemistry, and temperature. The plumbosolvency of a water (a measure of the extent of lead dissolution) is strongly affected by the pH and alkalinity of that water. Clearly the exposure to lead through drinking water, or through any food or drink for that matter, is also dependant on the quantity consumed. Drinking water can make up approximately 20% or more of an adults total exposure to lead, but may be as high as 85% for infants on formula mixed with tap water [18].

As well as ingestion through food and drink, lead may also be ingested through licking fingers after handling lead products or lead based paints, a problem particularly associated with children. Dust from lead based paints may also be inhaled or ingested where it has settled on food or kitchen surfaces. Exposures to lead dust may occur during mining, smelting, and refining of lead. Occupational exposure, which can often lead to toxic effects, is present in many other industries including manufacturing batteries, paints, glass, rubber, petrol as well as in the plumbing and printing industries.

Organic lead compounds have been used extensively as anti-knock and lubricating agents in petrol, but their use is now decreasing. However, the use of leaded petrol results in the emissions of lead into the atmosphere from traffic and industrial exhaust fumes [19]. Not only is this lead in the atmosphere a source of lead inhalation but it is also responsible for further contaminating the soil and water.

1.1.4 Sources of lead in drinking water

Due to its strength, durability and malleable characteristics, outlined previously, lead piping has been used extensively, throughout modern history, to connect drinking water supplies from water mains to peoples' homes. This has resulted in contamination of the water that is passed through lead piping, and the subsequent ingestion of lead present in the drinking water. Since the 1970s and 1980s, the use of lead piping for water supply has been phased out because of health concerns that were outlined in Chapter 1.1.2. Although lead pipes are no longer used in new plumbing installations, their presence in existing plumbing, installed prior to the 1980s, is still widespread today.

The primary source of lead in drinking water is through the dissolution of lead from the internal surface area of lead pipes [45,22]. However, lead can also enter drinking water through the leaching of brass and bronze fittings containing lead as well as through the use of lead in pipe jointing compounds and soldered joints. Galvanic corrosion of lead can occur when the metal is in contact with another such as copper. Such metallic coupling is most prevalent where lead containing solders were excessively applied to soldered joints between sections of copper pipework; this can produce high concentrations of lead until the lead from the solder has dissipated. Lead may also enter drinking water systems through lead that has been used in other plumbing components such as valve parts, fittings, fixtures, cisterns and linings for water tanks.

Another possible source of lead in drinking water is, rather curiously, through contact with unplasticized polyvinyl chloride (uPVC) pipes. This is caused by leaching of lead from the lead-salts that are sometimes used to stabilise the plastic in order to minimize thermal decomposition during extrusion. It has been shown [20] that lead stabilized uPVC can result in lead contamination of drinking water when very new. However, the contamination is short lived, and uPVC cannot be regarded as a significant source of lead contamination when compared to lead pipes [3].

Particulate lead content of drinking water has been suggested as one of the primary causes of extremely high lead levels occasionally found in drinking water. Particulate lead is thought to be caused by the flaking of fragile lead corrosion products from the inside wall of the lead pipe, though there is limited knowledge of the exact physical processes occurring here. Physical disturbances to the lead pipework, such as vibration from traffic, and water-hammer effects are thought to be the chief sources of particulate lead [21].

The research described within this thesis will focus primarily on the lead emissions to drinking water through lead pipes, since this has been found to be the chief source of lead contamination to drinking water [45,22].

1.1.5 The problem in the UK

In the European Union, as many as 40 to 50% of the houses in some Member States are believed to have a lead pipe, KIWA [22] having reported the best estimates (at the time) of the occurrence of lead plumbing for several countries in Europe, as shown in Table 1.1.

Table 1.1. Occurrence of lead plumbing in Europe.

Country	Properties with Lead Communication Pipes (%)	Properties with Lead Supply Pipes or Internal Lead Plumbing (%)
Belgium	19	15-30
Denmark	0	0
France	39	38
Germany	3	9
Ireland	50	51
Italy	-	5-10
Luxembourg	7	0
Netherlands	6	8
Portugal	?	32
United Kingdom	**40**	**41**

The use of lead pipes to plumb newly built houses into the water supply system was phased out in the early 1970s in the UK because of health concerns, such concerns now being confirmed by epidemiological evidence [23]. However, many properties in the UK were built prior to 1970, and, consequently around 40% are still supplied through old lead pipe, as highlighted in Table 1.1.

In many cases, this lead pipe is the communication pipe, i.e. the pipe that connects the water mains to the internal plumbing and is usually partly owned by the water company and partly owned by the consumer. The communication pipe usually runs several feet underground from the road, where it connects to the water main, to the internal plumbing in the house, making it far harder to remove than the internal plumbing in the house. In 1990 the DoE undertook a survey [24] to establish the proportion of properties that still had lead communication pipes or internal lead plumbing, for different regions in England and Wales. The survey revealed that in the South East, approximately 19% of households are supplied through lead communication pipes, and approximately 8% of households have internal lead plumbing. This is in marked contrast to the survey results for the North West; where approximately 62% of households are supplied through lead communication pipes, and approximately 75% of households have internal lead plumbing.

1.1.6 Drinking water standards

Drinking water supplied by water companies must not contain toxic substances, such as lead, that can cause detrimental health effects. The Government has set legal standards, relating to the concentrations of such substances, for drinking water in the Water Quality Regulations [25]. Most of these come directly from an obligatory European Community Directive but some UK standards are more stringent. The majority are taken from the drinking water standards recommended by the World Health Organisation (WHO) [26]. The Drinking Water Inspectorate (DWI) is then responsible for ensuring that the water companies in England and Wales supply water that is safe to drink and meets the standards set in the Water Quality Regulations.

In the last thirty years, the standards and guidelines for lead in drinking water have tightened considerably due to the growing epidemiological evidence of the adverse health effects of lead, particularly in young children. The first guidelines for lead in drinking water were set in the first edition of WHO International Standards for Drinking Water in 1958 where a general limit of 100μg/l was set [27]. In 1961 WHO published the first edition of the European Standards for Drinking Water, the purpose of which was to encourage the more advanced European countries to attain higher standards than those previously recommended by WHO. However, the set limit for lead in the European Standards for Drinking Water remained at 100μg/l, although a clause was added, which stated that 'In no instance should the concentration of lead (as Pb) exceed 0.3mg/l after 16 hours' contact with the pipes. If the limit of 0.3mg/l is regularly exceeded it will be necessary to take steps either to change the piping or to treat the water [28]. These standards remained unchanged in the second edition of the European Standards for Drinking Water, published in 1970.

This standard remained in operation in the UK until 1980 when the "directive relating to the quality of water intended for human consumption" of the European Community (EC) [29] was adopted. This "drinking water" directive specifies a limit of 50μg/l for lead in drinking water, this time being applied as a Maximum Admissible Concentration (MAC) in a running water sample, i.e. from a fully flushed water system. A clause to this standard stated that if a MAC of 100μg/l, in a running water sample or in a sample taken directly, was frequently exceeded or exceeded to an appreciable extent, then remedial action must be taken.

In 1984 WHO published Guidelines for Drinking Water, which recommended a limit of 50µg/l for lead in drinking water, based on maximum concentration. However, the lead standards in the UK would continue to be based on the EC "drinking water" directive until the 1989 and 1990 Water Acts were adopted. These acts specify a MAC of 50µg/l of lead in drinking water for any water sample taken; this standard being applied to the present day (2003).

In 1993, WHO revised its guidelines for lead in drinking water and recommended a value of 10µg/l (as Pb) based on a tentative limit for average weekly ingestion. The recently revised (1998) European Union "drinking water" directive [30] has recognised this guideline and requires Member States to comply with an interim lead standard of 25µg/l by December 2003 and then 10µg/l by December 2013, these limits being related to the weekly average concentration at individual properties. The Directive requires compliance samples, in respect of the lead parameter, to be taken from the point of use by consumers (normally taken to be the kitchen tap), although a harmonised sampling method has yet to be specified.

Similar standards, often based on WHO guidelines, have been set in other European countries as well as in the USA. In the case of the United States, the standard for lead in drinking water is specified by the Lead and Copper Rule [31], first proposed in 1991 by the USA Environmental Protection Agency. Although this regulation is complex, the general standard set for lead in drinking water is 15µg/l at the 90th percentile, based on 6-hour stagnation samples taken from reference houses.

1.1.7 The new EU directive

The revised "drinking water" directive [30], which came into force on 25 December 1998, requires an interim standard for lead of 25µg/l to be achieved by 25 December 2003, and a final standard of 10µg/l to be achieved by 25 December 2013. A note associated with these standards indicates that these parametric values apply to a sample of water intended for human consumption (that is from the consumer's tap) obtained by an adequate sampling method and taken so as to be representative of a weekly average value ingested by consumers. The European Commission has indicated that it intends to provide guidelines on harmonised sampling and monitoring methods, which Member States will be required to follow, however, these have not yet been agreed upon [32].

In the case of domestic premises, Member States will be deemed to have fulfilled their obligations where it can be established that non-compliance with the parametric values for lead with the standards at these taps is due to the domestic pipework owned by the consumer. However, in the case of premises and establishments where water is supplied to the public, such as libraries, schools and restaurants, compliance with the standards is required at the taps normally used for human consumption [33].

If there is a risk that water supplied to a domestic property will not comply because of the domestic pipework, then, from Article 6(3) [30] Member States must ensure that the appropriate measures are taken to reduce or eliminate the risk of non-compliance. This may involve the application, by the water supplier, of alternative or additional measures, such as appropriate treatment techniques to change the properties of the water before it is supplied to the consumer. When treatment does not achieve compliance, the water supplier must replace (or reline) the lead service pipes it owns, which connect the consumer to the water supply, advising or informing the consumer of any additional remedial action they should take. These actions are clarified further by Note 4 to Part B of Annex 1 [30], which states 'Member States must ensure that all appropriate measures are taken to reduce the concentration of lead in water intended for human consumption as much as possible during the period needed to achieve compliance with the parametric value' (i.e. both 25 and 10μg/l). Note 4 then states: 'When implementing the measures to achieve compliance with that value Member States must progressively give priority where lead concentrations in water intended for human consumption are highest'.

It can be concluded from the wording of this Directive that corrective water treatment is required until all lead pipes have been removed, including those owned by householders. Simply advising householders to remove their lead pipes (assuming the water company removes theirs) or to flush the pipe work prior to use for consumption is not a realistic proposition. At least in the UK, most householders do not wish to replace their lead pipes because of the cost and the inconvenience and it is unlikely that householders will remember to flush their pipes once the novelty has soon worn off [34].

In order to demonstrate compliance with the new standards, it is stated that water suppliers must obtain water samples by an adequate sampling method, taken so as to be representative of the quality of water consumed throughout the year. Note 5 to Table B1 of Annex II [30] states: 'As far as possible, the number of samples should be distributed equally in time and location'.

1.1.8 Complying with the new directive

In order to comply with the lead standards specified in the new "drinking water" directive, all water suppliers are required to have a strategy of action to meet the interim and final lead standards. This will involve corrective water treatment, to reduce the plumbosolvency of the water supplied, as well as strategic lead pipe replacement where required. The DWI has advised water suppliers, in an Information Letter [33], that they will need to consider additional treatment or optimisation of existing treatment when more than 5% of samples exceed 10μg/l in the water supply zones (i.e. the rural or city districts) they supply. The DWI have suggested a general timetable [33] for water suppliers in order to comply with the timetable required by the "drinking water" directive, Ministers, and the Water Supply (Water Quality) Regulations 2000 [25]. This states that

- 'all new and further plumbosolvency treatment measures required to attempt to meet the 10μg/l standard must be installed and commissioned by 31 December 2002 and optimised for 10μg/l by 25 December 2003;
- where necessary, existing plumbosolvency treatment measures must be optimised for 10μg/l by 31 December 2002;
- after plumbosolvency treatment has been optimised, any strategic lead pipe replacement required to meet 25μg/l must be completed by 25 December 2003; and
- after plumbosolvency treatment has been optimised, any strategic lead pipe replacement required to meet 10μg/l must be completed by 25 December 2013.'

1.1.8.1 Lead pipe rehabilitation and replacement

Ideally, to reduce the lead content in drinking water as much as possible, all lead pipework, used for the supply of drinking water, should be replaced by pipes of an alternative material, e.g. plastic. At present, the Netherlands is the only country to have elected to replace all of its lead pipes. This is a much more viable option than in the UK because the Netherlands has far fewer lead pipes (Table 1.1) and 100% grant aid is being provided by the Dutch Government.

The cost of replacing all lead pipework in the UK has been estimated at approximately £10 billion [19,45]. Since the lead pipe present in the UK is partly owned by water suppliers and partly owned by consumers, the total cost would be split, with approximately £2 billion for UK water companies and £8 billion for consumers [19]. Across Europe the cost of replacing all the lead pipes is likely to be in excess of £80 billion [34]. The other major drawback of widespread lead pipe replacement is the disruption it would cause, particularly in town and city centres. Such schemes would impose great restrictions on much of the road network and greatly affect the traffic system for extended periods.

It is clear, from these points, that any lead pipe replacement will have to be selective and strategic, this will usually be where lead concentrations in consumer's drinking water are highest and where lead standards in establishments where water is supplied to the public, e.g. schools and libraries, are breached. However, the DWI has also indicated that it would 'welcome proposals for opportunistic lead pipe replacement, particularly where synergy can be gained in conjunction with the "quality-driven" mains renovation programme', however, these will need to be justified [33]. Although partial lead pipe replacement by water suppliers is widely advocated, it has been shown to be deeply flawed [35], since the resulting disturbances to the remaining lead pipe can often increase lead emissions in drinking water, as well as being very costly.

There is only one suitable pipe rehabilitation technique available to reduce or eliminate lead emissions to drinking water from existing lead pipes. This technique is known as slip lining and involves the insertion of a rubber sheath to the inside of the lead pipe. The sheathing simply acts as a barrier between the water and the lead pipe, effectively eliminating further dissolution of lead into water. However, it should be noted that this technique is often costly and can be dependant on pipe conditions [36,37].

1.1.8.2 Water treatment

The preferred approach to meet the tighter water standards in the UK, currently employed by most water suppliers, is to install or improve remedial water treatment before it is supplied to the consumer. This is because it is highly cost effective and does not involve any disruption to existing pipework, providing comprehensive protection so that public health objectives can be met without requiring consumers to take action themselves. There is also a great deal of experience in the use of corrective water treatment to reduce lead emissions from lead pipes in the UK and United States, which dates back to the 1970s [3,38,39,40,41].

Corrective water treatment involves altering the properties of the water being supplied to the consumer in order to reduce its plumbosolvency and thus reduce the lead emissions. Initially this was carried out, where necessary, simply by raising the pH and in some cases increasing the alkalinity (calcium carbonate content) of the water. The control of pH is effective in the case of low alkalinity, low pH waters since it limits the solubility of lead carbonates (the lead corrosion products). However, in the case of high alkalinity waters, pH adjustment has no effect, consequently alternative treatment methods are required.

As well as the control of temperature and pH, a number of chemical treatment techniques have been investigated [42], the most effective of which has been found to be the dosing of phosphate (a corrosion inhibitor) at an appropriate pH. Phosphate, usually dosed as orthophosphoric acid, reacts with the lead to form a highly insoluble compound on the inside surface of the pipe, which acts as a barrier and helps to prevent lead dissolving from the pipe into the water. Extensive research into the long-term effects of phosphate dosing on lead emissions, as well as investigating the optimum dosage of phosphate as a corrosion inhibitor, has been carried out for a range of different water types [43]. This has indicated [44,45] that once optimised, phosphate dosing at an appropriate pH will probably achieve the interim 25μg/l lead standard in most of the UK without the need for lead pipe removal, and will achieve the 10μg/l lead standard for the majority of the UK, albeit possibly in conjunction with selective lead pipe replacement. The DWI has recognised this and has stated, in an Information Letter [33], that 'where orthophosphate is dosed, it must be dosed at the optimum orthophosphate concentration and the pH value within distribution maintained within the optimum range. The optimum orthophosphate concentration must be maintained and stabilised as far as practical within the distribution system'.

Research findings have shown that higher doses of phosphate are required for waters of higher alkalinity, and the general dosage range is about 1.0 to 2.5mgP/l [45]. The environmental impact of such low phosphate doses is not significant when sewage already contains much more phosphate from human waste and detergents. Laboratory plumbosolvency testing [38,43,46] has also revealed that the optimum pH for phosphate treatment is 8.0 to 8.5 for low alkalinity waters and that pH is much less important in the phosphate treatment of high alkalinity waters.

1.1.9 Assessing compliance

In order to demonstrate that the required level of compliance with the new lead standard has been achieved, water suppliers are required to monitor lead emissions in water samples taken from the area that they supply. Additionally, compliance assessment is also essential for demonstrating the optimisation of corrective water treatment, though operational control requires more data. As described previously, the new "drinking water" directive indicates that the parametric values of 10μg/l and 25μg/l apply to a sample of water intended for human consumption (that is from the consumer's tap) obtained by an adequate sampling method and taken so as to be representative of a weekly average value ingested by consumers [32]. To date, there are no indications that a specific harmonised monitoring protocol, in order to enable a straightforward and uniform implementation of the new directive, will be agreed upon. However, there are a number of options available to water suppliers for assessing compliance; these include a range of sampling techniques.

1.1.9.1 Sampling methodologies

In order to assess the exact compliance with the new lead standards, it would be necessary for the water supplier to measure the lead emissions at the tap every time the tap is turned on, for every single consumer to which they supply water. Note that in order to take into account the seasonal variation of temperature, which effects lead emissions [60,61], this must be carried out over the course of one year. Clearly this is not feasible considering the huge cost and time burdens such a scheme would entail. A more practical solution, which has been extensively employed by the UK water industry for many years, is to use sampling methods. These generally involve the collection of a water sample from randomly selected properties served by the water supplier.

1.1.9.1.1 Composite proportional sampling

Arguably the most accurate of sampling techniques, for the measurement of weekly average concentration of lead ingested by consumers, is composite proportional (COMP) sampling. This involves the installation of a device, by the water supplier, which connects to the kitchen tap at a number of randomly selected properties served by the water company. Whenever water intended for human consumption or for cooking is to be used, the consumer must turn a "split-off" valve, which directs 5% of the water drawn from the tap into a sample bottle. This procedure must be carried out for an entire week, after which the COMP device is removed and the water sample collected is analysed for lead content by the water supplier.

Although the lead content of the water sample collected through the COMP device may not be representative of all of the houses supplied by the water company, it is clearly representative of the weekly average value ingested by consumers at the house where it was installed, and takes account of all variations in lead emissions during the test period. However, despite its accuracy, water suppliers seldom use this technique since it is highly costly and time consuming. Moreover it is an intrusive technique, which, not only requires the installation of a device at the tap but also places great demand on the consumer to turn the "split-off" valve every time water is used for drinking or cooking. For these reasons it has been stated [22] that 'In itself, the composite proportional sampling procedure is a long-term test, which is not appropriate for large scale and routine monitoring', however, the technique does offer a sound means for investigating specific problem circumstances

1.1.9.1.2 30 Minute stagnation sampling

The most widely used "fixed stagnation time" sampling method is 30 minute stagnation sampling (30MS). This is because the procedure was believed to emulate the typical water usage that occurs at a house, i.e. a mean inter-use time of 30 minutes, and so reproduce the likely lead concentration in water drawn from the tap. The 30MS procedure involves randomly selecting a property from the supply area. The plumbing system is then flushed for 5 minutes at 5 litres/minute by running water through the tap to be sampled. The water is then allowed to stand (stagnate) for 30 minutes, making sure that no water is used from the internal plumbing system, including alternative taps and toilets, during this time. After exactly 30 minutes the first litre from the tap is collected into a sample container without flushing the pipe beforehand; the sample is then analysed for lead content by the water supplier.

While this technique has been proven to be reproducible at a single property [47], by virtue of isolating all the variables associated with lead emissions, it is not as representative as COMP because it does not take into account real water use. Although some studies [47] have shown 30MS to be representative of lead emissions at the property sampled, it can be demonstrated that the 30MS result is governed by the plumbing circumstances at the property due to dilution effects. As with COMP sampling, 30MS sampling is expensive and time consuming. The procedure also causes considerable intrusion, albeit for only 30-40 minutes, since the consumer cannot use any water during this period of time.

However, the DWI has indicated a clear preference that samples (30MS) should be taken at a small number of specially selected (fixed) properties that have a lead pipe, or at lead pipe rigs placed at appropriate points in the distribution system, to monitor the effectiveness of plumbosolvency treatment measures they have taken [32,33].

1.1.9.1.3 Random day time sampling

The most widely used sampling technique, employed by water suppliers in the UK, is Random Day Time (RDT) sampling. This approach has been used extensively for assessing compliance with lead standards since 1989 and remains the most favoured protocol in terms of costs, practicality and consumer acceptance. RDT sampling involves the taking of a one-litre sample directly from the kitchen cold-water tap of a randomly selected property at a random time during the working day (i.e. between 9am and 5pm), without flushing any water beforehand.

RDT sampling is simple, practical, and relatively inexpensive and is the least invasive method since the entire procedure can be carried out in a few minutes. However, although some studies [47] have found RDT sampling to be representative of the average lead emissions that occur at single houses, the procedure is not reproducible due to the variation in stagnation time throughout the day as a consequence of the water usage.

The DWI has proposed that water suppliers continue to use RDT sampling as a method of assessing compliance with the lead standard and recognises that this method may overestimate the number of failures to meet the standards compared with the more accurate COMP sampling [32]. The use of RDT sampling for the purposes of optimising plumbosolvency control is still favoured by some water suppliers because it is less inconvenient for consumers, less costly and samples can be taken in conjunction with the more extensive bacteriological monitoring that is carried out. However, because it is believed [22,48] that RDT sampling is not sufficiently reproducible, the DWI will only permit a water company to use RDT sampling for the purposes of optimising plumbosolvency control if it can be demonstrated that such sampling is equivalent to the monitoring of fixed reference points. The DWI has also stated that 'water companies should bear in mind that random daytime samples are much more variable than stagnation samples' [32].

1.1.9.2 Limitations of sampling

In the UK water industry, RDT sampling is the preferred approach for assessing compliance with the lead standards, due to its low cost, simplicity, practicality and high customer acceptance. However, as previously discussed, it suffers from some major disadvantages, namely poor reproducibility. This is caused by the wide variation in lead emissions that can be expected at a single property over the course of the day, which, in turn, is related to the way that the water is used by the consumer. Thus, RDT samples taken from the same house will usually be different to some extent. This problem of poor reproducibility is compounded across a water supply zone since the circumstances relating to lead at individual properties differ widely, greatly increasing the difficulties associated with the assessment of the extent of the lead problem.

In order to more accurately quantify this wide variation of RDT sampling results, and thus improve the reproducibility of the sampling procedure on a zonal scale, it is necessary to take a higher number of RDT samples. Clearly more sample results equates to a better representation of the water supply zone. Although RDT sampling is cheaper and less time consuming than any other sampling method, it nevertheless puts considerable demands on the water supplier. Therefore, only a limited number of RDT samples can realistically be taken by the water supplier.

In respect of the lead parameter, the minimum sampling frequencies specified by the UK Water Supply Regulations [25], which implement the Directive, vary from only 1 to 8 samples per year from each water supply zone, dependant on the population involved (up to a maximum of 100, 000 people). As well as water supply zone size, the number of samples required to get an accurate assessment of compliance has been found to be dependant on the range of variation of lead levels found in that area and the true level of non-compliance in that area. [22] It is widely recognised that such frequencies are far too low for accurate assessments to be made. However, the random daytime sampling of water supply zones is more comprehensive in respect of assessing compliance with bacteriological standards, the minimum specified sampling frequencies varying from 120 to 240 per year for zones up to 100,000 people. Thus, water supplies have often taken RDT samples for monitoring compliance with the lead standard in conjunction with the more extensive bacteriological monitoring that is carried out. It is also possible for water suppliers to analyse large conglomerates or RDT sample data relating to the lead standard, collected over a period of several years.

With respect to optimising plumbosolvency control, the use of RDT sampling may be possible where large numbers of samples have been taken. However, it is thought that whilst RDT sampling may be adequate to measure large improvements from corrective water treatment, it will become increasingly difficult if not impossible to differentiate the effects of further corrective treatment where the improvements are subtler, even with large numbers of samples.

1.1.9.3 Computer modelling

The uncertainty inherent in RDT sampling results brings into question its function as a reliable tool for the monitoring of compliance with the lead standard and assessment of the effects of further corrective treatment. Without adequate quantification of zonal compliance, the prioritisation of further corrective actions becomes more speculative and prone to error. This undermines the ability to justify these actions, to minimise their costs, and to demonstrate their success. Computer simulation of household lead emissions offers the possibility for achieving a greater understanding of the issues that relate to plumbosolvency control. Consequently, the DWI has stated that, where appropriate, computational models can be used in the optimisation of plumbosolvency treatment and control [33].

Over the last 20 years, significant advances in predicting both lead emissions at the tap, and compliance, with respect to the lead standard, for a water supply zone, have been made [49,50,51,52,53,72]. Some of the most significant work include the simulation of lead released during stagnation, flow within a pipe, and estimation of the daily average concentration of lead at a single property. With particular interest for water suppliers, methods of simulating compliance sampling on entire water supply zones, with particular emphasis on RDT sampling have also been developed [53].

In most cases, experimental data has been obtained to substantiate the models predictions; validation has generally been reasonable. Bailey and Russell [49] predicted average concentration of lead at the tap for one day, at an individual property, by combining assumptions based on water usage with the basic characteristics of lead dissolution in a pipe. Similarly, Clement [52] uses simplistic water pattern data to determine the mass of lead ingested per person per day by weighting the concentrations predicted for a range of stagnation times by the approximated corresponding volume of water used after these stagnations. More sophisticated models, based on more accurate mathematical descriptions of the physical processes that take place in a lead pipe, have been developed [50,51]. However, these models are limited in that they have only been able to predict lead emissions during stagnation or during flow as opposed to daily average lead emissions at a property.

With the exception of Hayes et. al. [54,61], with whom the author has collaborated, the only example of computational modelling of compliance data for a complete water supply zone is that developed by Cardew [53]. Cardew has attempted to simulate the process of RDT sampling within a water supply zone. Here, the structure of a complete water supply zone is simulated by randomly ascribing parameters such as pipe lengths and water parameters for individual properties from distributions that describe the entire zone. The purpose of the random ascription of these house circumstances is to mimic the extent and shape of the wide variation that occurs across real water supply zones. A stagnation time is randomly selected from a Poisson distribution for a randomly selected property within the simulated zone. The concentration of lead in the drinking water contained within the lead pipe is then readily calculated using basic characteristics of lead dissolution in a lead pipe. However, Cardew assumes that the concentration of water within the lead pipe at the start of the stagnation period is completely free of lead. This assumption has to be made since this method does not take into account the water usage, and therefore lead concentration within the pipe, throughout the day up to the point of taking the sample. The 1-litre sample concentration is estimated by use of simple dilution factors based on lead pipe volume, non-lead pipe volume, and sample volume. Due to its simplicity, this method is computationally very fast.

1.1.10 Research objectives

In light of the limitations of traditional sampling methods, for use in assessing compliance with the new lead standards and optimisation of further corrective treatment, previously discussed, alternative methods are required. In particular, the use of computational models, to investigate the issues that relate to plumbosolvency control, can provide a valuable tool to water suppliers. However, to date, the majority of the models developed have been of limited use, since they are only able to predict average lead emissions at a single property, or lead emissions during an individual stagnation or flow event. Although there is currently one example of a computational model that can assess compliance for a complete water supply zone, it is of limited flexibility since it can only predict zonal compliance based on the RDT sampling method. It should be noted that this existing "zonal model" is not capable of simulating lead emissions at an individual property, and does not fully model the flow or mass transfer processes that take place within a lead pipe.

These limitations of existing computational models have provided the motivation to develop a more complete model, for use, by water engineers, to assess compliance and facilitate the optimisation of corrective treatment. With the continuing progress of new technology, personal computers are becoming fast enough to solve highly complex problems in a matter of seconds. It is clear that this vastly increased processing power could be harnessed to run a more complex computational model than those previously developed. Prior to the development of such a model, it is first necessary to outline the primary features and capabilities the model must possess. The main practical consideration is that the model must be developed to suit the needs of a water engineer, who may have limited computer knowledge and will likely have modest computing resources, i.e. will have access to a standard PC rather than a supercomputer.

The capability to model lead emissions, over the course of an entire day, at a given property, is paramount for investigating how parameters, such as pipework and water usage, effect the lead emissions, both as a daily average value and at various times throughout the day. In order to accurately model lead emissions at a single property throughout the day, it will be necessary to employ more precise mathematical descriptions of the physical processes taking place within the system; these processes include the fluid flow and mass transfer within the pipework.

The capability to model the structure of an entire water supply zone is necessary for predicting zonal compliance with the lead standard as well as for investigating the likely effects of corrective water treatment and selective lead pipe replacement. This is intended to facilitating the optimisation of plumbosolvency control measures and substantially overcome the severe limitations of traditional sampling. Additionally, a detailed description of the simulated water supply zone will allow greater understanding of the likely characteristics of problem properties, where lead emissions will be highest. The ability to model the daily average concentration of lead for a single property can be extended to an entire water supply zone, resulting in a prediction of the zonal compliance with the lead standards that is completely representative of the weekly average value ingested by consumers.

The capability to simulate various sampling protocols will also be necessary in order to characterise the behaviour of a simulated zone in a way that can be validated to the data collected by the water company. This will also enable various different sampling protocols, which are currently employed by water companies, to be evaluated in terms of how accurately they predict actual compliance, i.e. how representative they are, and how suitable they are for use in the optimisation of corrective treatment. Of particular importance will be the ability to simulate RDT sampling, since this is currently the most widely employed method of assessing compliance in the UK. As a consequence, it will be possible to investigate the reproducibility and possible variation in results of this sampling method by repeatedly simulating RDT sampling surveys.

1.2 The real-world problem

1.2.1 Solubility of lead in drinking water

1.2.1.1 Chemistry

The lead content of drinking water that has been in contact with lead pipes is highly dependant on the chemistry of the particular water. Chemical characteristics of drinking water vary considerably throughout the U.K., from soft acidic waters in the North West to hard chalky waters in the South East. Consequently, lead solubility, and hence compliance with the new lead standards, has the potential to be highly variable throughout the U.K.

The chemical reactions between the water and the inner surface of the lead pipe determine the solubility of lead in the drinking water. It is important to note that the term solubility describes the maximum concentration of lead in drinking water possible under the set chemical conditions. This maximum (or equilibrium) concentration is achieved when the chemical system is in equilibrium and no more lead can be dissolved into the water. This 'equilibrium' concentration is typically achieved between 8 and 24 hours, depending on pipework diameter, for drinking water stagnating in a lead pipe.

Although the internal surface of unused (fresh) lead pipes has a bright lustre, this disappears soon after the pipe is used to supply water. Under the redox conditions (a measure of chemically oxidising or reducing potential) that are normally encountered in drinking water, elemental lead is unstable and oxidises to form lead (Pb^{2+}) ions, that is, the metal corrodes. The lead ions so formed dissolve and/or react with constituents of the water (such as carbonate) and precipitate as a solid, which is normally found as a deposit on the internal wall of the lead pipe. This deposit of corrosion products forms a layer, which inhibits further corrosion to some degree [55]. The layer of corrosion deposit is sustained by continuing metallic oxidation as influenced by the corrosivity of the water flowing through the pipe.

The solubility of lead in water depends on the composition of the water, particularly pH, ionic strength, the concentration of carbonate, and the redox potential, all of which determine the species of lead in solution and the solid that precipitates. The Pb^{2+} concentration at equilibrium can be calculated simply by using the solubility product expression for the solid. The solubility product, used in this expression, is the equilibrium constant that describes the reaction by which a precipitate dissolves in pure water to form its constituent ions. The solubility products for various solids have been found by experiment and most published values are for equilibrium at 25° C. It is worth noting that the solubility product, and hence solubility, can be significantly affected by temperature of the water; this is the reason why lead emissions are lower in winter than in summer. As a general guide, lead concentrations tend to be about twice as high in the summer than in the winter.

However, this simple approach does not take into account the fact that Pb^{2+} ions associate with anions, which act as ligands to form soluble complexes or ion pairs, increasing the total dissolved lead concentration, in some cases by orders of magnitude [55]. Examples of ion pairs/complexes involving lead are shown below:

$Pb^{2+} + H_2O = PbOH^+ + H^+$
$Pb^{2+} + CO_3^{2-} = PbCO_3$
$Pb^{2+} + Cl^- = PbCl^+$
$Pb^{2+} + H^+ + PO_4^{3-} = PbHPO_4$

The total concentration of lead in solution is given by the sum of the concentrations of all dissolved lead species and these are determined by a series of interacting equilibria involving the major dissolved components in the water, the lead solid and these dissolved lead species (free aquo ion, ion pairs and complexes). Hence, the calculation of the total dissolved lead concentration requires the solution of many simultaneous equations describing these equilibria [55].

Lead carbonate is the most stable corrosion product in such circumstances because of the relative solubilities of all the lead compounds that could be formed and two forms of lead carbonate are found:

[1] normal lead carbonate (cerrusite) ... $PbCO_3$
[2] basic lead carbonate (hydro-cerrusite)... $Pb_3(CO_3)_2(OH)_2$

The reason why basic or normal lead carbonate should form is not fully understood, although the total ionic composition of the water appears to be relevant. It is significant which form of lead carbonate is present since they have different solubilities, which are strongly influenced by the pH of the water [21]. The solid that produces the lowest solubility under given conditions will be the most stable solid phase in that instance. However, the examination of pipe deposits has shown many cases where the more soluble (but thermodynamically less stable) solid hydro-cerrusite occurs where cerrusite is predicted. Although thermodynamics predicts that only one of the lead carbonate solids should exist at equilibrium, both solids are often found at the same time [39]. Figure 1.1 shows the general relationship of lead carbonate solubility with pH and alkalinity.

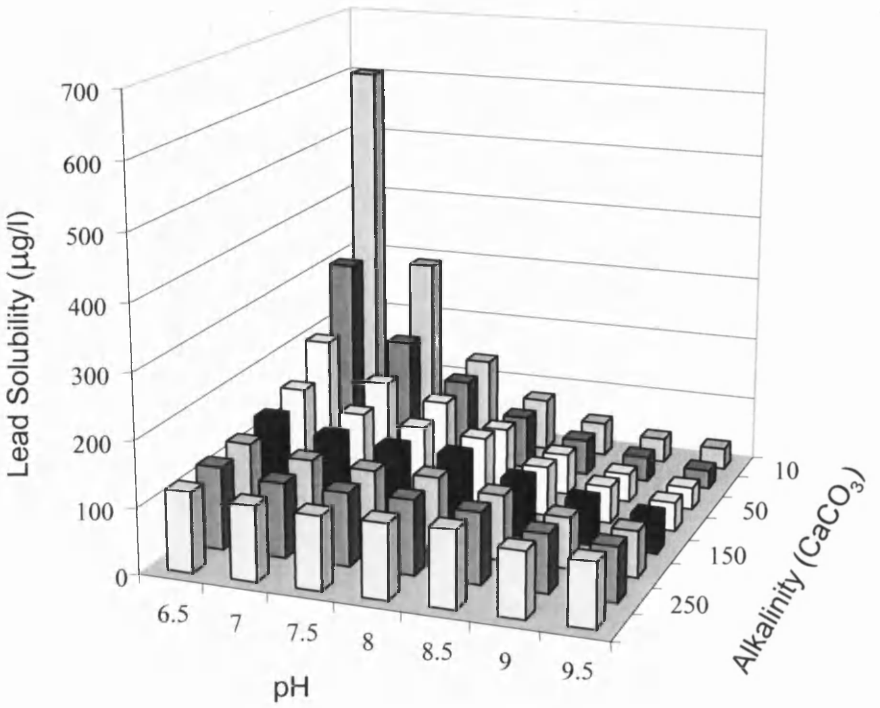


Figure 1.1. Lead solubility as a function of pH and alkalinity.

The organic content of the water has also been shown to strongly influence the solubility of water, the presence of naturally occurring humic and fulvic acids increasing the amount of lead dissolved into the water. Although not proven, this phenomenon is likely to be explained by some form of organo-metallic complexation. The nature of the corrosion deposit could also be influenced by the deposition of calcite (calcium carbonate) in "hard water" areas and by iron corrosion products [21].

As discussed previously, corrective water treatment that is used to achieve reductions in plumbosolvency, necessary to achieve compliance with the lead standards, often takes the form of orthophosphate dosing. The resulting solid that is precipitated is lead phosphate, which is far less soluble than lead carbonate and soon dominates the corrosion deposit within the lead pipe. The most likely forms of lead phosphate are considered to be $Pb_5(PO_4)_3OH$ (hydroxypyromorphite) and $Pb_3(PO_4)_2$ (tertiary lead orthophosphate) [21].

1.2.1.2 Solubility modelling

The solubility of lead in a particular water can be estimated through solubility modelling if the water's composition is known. In order to model the solubility of lead as accurately as possible it is necessary to consider all of the possible lead species that could arise, which, in turn, are determined by the chemical composition of the water. Estimation of lead solubility is then carried out by solving the mathematical equations that describe the interacting chemical equilibria involving the major dissolved components in the water, the lead solid and the dissolved lead species. The most detailed solubility models [55,56,57] consider many possible water constituents, which results in a large number of non-linear simultaneous equations. In order to solve these complex systems it is often necessary to employ numerical methods. The use of computers also facilitates the computation of lead solubility over the full range of water conditions likely to occur.

A relatively simple computer model, to predict lead solubility in drinking water, has been developed to show the detailed response of the theoretical solubility curves for lead to changes in dissolved inorganic carbonate concentration C_t and pH at 25° C. Considered were lead carbonate complexes, lead hydroxide monomers and polymers, the free Pb(II) ion, and the possible solids that could precipitate (lead hydroxide, normal lead carbonate, basic lead carbonate). The resulting solubility estimates are plotted over a pH range for three different carbonate concentrations, assuming a fixed ionic charge of 0.1 (Figure 1.2).

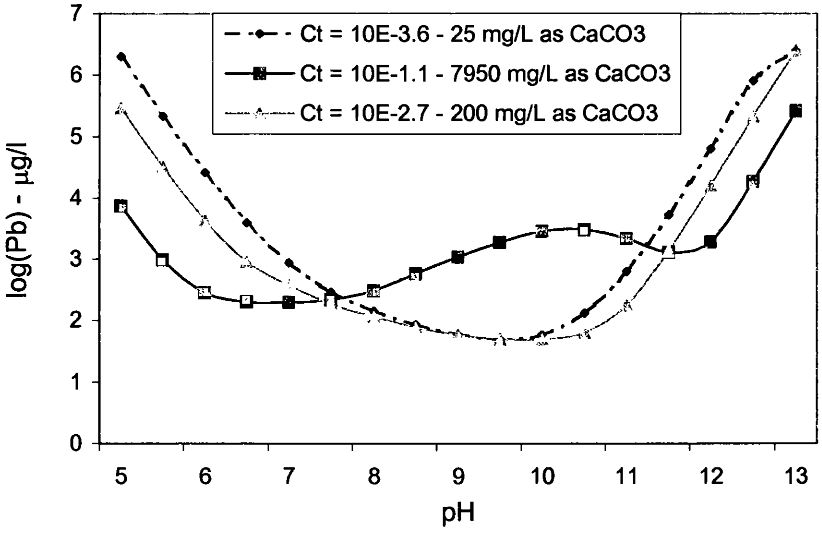


Figure 1.2. Solubility as a function of water quality.

Although solubility modelling can be a useful tool for investigating the general relationships between water quality and solubility, they are still subject to large uncertainties due to the lack of accurate equilibrium data. Organic quality can influence a water's plumbosolvency, often increasing the solubility of lead significantly and reducing the effects of phosphate dosing [38,58]. However, the specific effects of organics, often present as the humic and fulvic acids associated with organic colour, on lead solubility is still not fully understood and there is limited data on complexes of lead with natural organic materials such as humic substances. It is only recently that solubility models have incorporated a factor for organic constituents [59] and such adjustments to solubility predictions are unlikely to be anything more than an approximation because of the complexity and variability of the organics involved.

1.2.2 Measuring plumbosolvency

The solubility of lead in drinking water can be estimated using solubility modelling as previously discussed. However, a more accurate approach of characterising the plumbosolvency of a water is to physically measure the concentration of lead within the water after it has been standing in a lead pipe. This method, which can be readily carried out in a laboratory, overcomes the problems associated with solubility modelling and can provide more detail about the plumbosolvency of a water.

Solubility modelling can predict the solubility of lead in water at equilibrium conditions only, i.e. the maximum or 'equilibrium' concentration of lead in drinking water. This is effectively when 'no more lead can get into the water'. However, in real life these 'equilibrium' conditions are rarely achieved in a consumer's plumbing system, because the time it takes to achieve this is far greater than the average time between water usage, even if the water is used infrequently. Typically, the only time the lead dissolution reaction gets close to achieving the 'equilibrium' condition is when the water has been standing in the pipes overnight. Thus, it is far more useful to quantify the variation of lead concentration over time for water stagnating in a lead pipe.

The simplest approach to quantify this variation is to measure the concentration of lead in water samples taken from a lead pipe after different stagnation times (periods of zero flow). The resulting time – concentration response accurately characterises the plumbosolvency of the water for that particular diameter lead pipe. In most cases this response has been found to follow a typical 'logarithmic decay' type curve that asymptotes to the 'equilibrium' concentration. This is known as the stagnation curve, an example of which is illustrated (Figure 1.3). Generally, for 12mm internal diameter lead pipes, lead concentration in water has been found to be at least 90% of the 'equilibrium' concentration after 12 hours of stagnation.

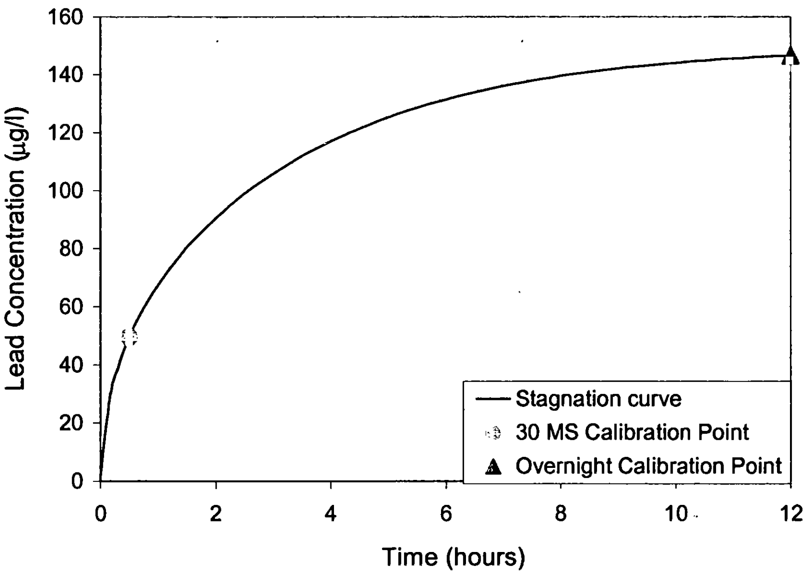


Figure 1.3. Stagnation curve showing how lead concentration increases over time.

A straightforward laboratory method of measuring plumbosolvency was developed in the 1980s by Colling et al. [43], which followed on from earlier work by Sheiham and Jackson [39], and has been widely used in the U.K. since. It involves the pumping of a test water, at a low flow rate, through short sections of pre-cleaned lead pipe, under standardised laboratory conditions. The flow rate is set so that the water-lead contact time is 30 minutes, and samples of the water are then analysed for lead content. Additionally, an overnight standing result is obtained at the end of the testing period. Since the general response of the lead dissolution system, i.e. shape of the stagnation curve, is known, the 30-minute stagnation (30MS) test result and the overnight test result can be used as calibration points as illustrated (Figure 1.3).

The complete testing of a particular water usually takes 3 to 4 weeks, during which the lead emissions are measured about 10 times. After a decrease from initially higher concentrations at the start of the test, stable lead values are normally obtained after approximately one week (Figure 1.4). This is due to the formation of a corrosion deposit, e.g. lead carbonate, on the inner wall of the lead pipe in the first week, which inhibits further corrosion to some degree. Throughout the test, the lead pipes are kept at a fixed temperature of 25 degrees C to represent the maximum likely temperature for lead pipes in the U.K., and thus produce the maximum likely lead emissions that would be encountered. This temperature also provides useful acceleration of the test.

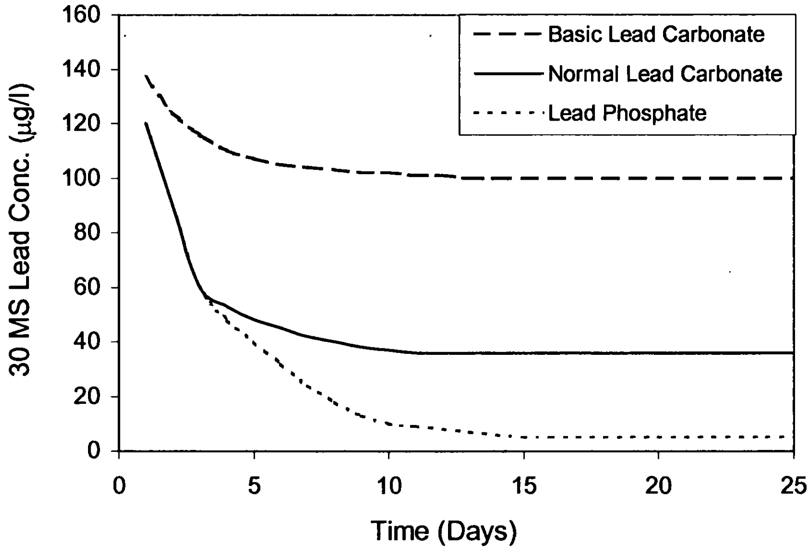


Figure 1.4. Typical results from laboratory testing.

Laboratory testing provides another advantage over solubility modelling in that it inherently accounts for any organics that may be present in the water by virtue of being based on direct measurements from that water. Laboratory testing has also been strongly endorsed by the DWI as a preferred method for helping to optimise plumbosolvency control treatment, in particular, to 'make an estimate of the optimum orthophosphate dose and optimum pH value' [33]. This can readily be achieved by making simple chemical additions to a series of water samples from a particular source, and performing the laboratory testing procedure on each.

1.2.3 Factors effecting household lead emissions

The concentration of lead in drinking water varies both throughout the water supply zone and throughout time. This is because lead emissions are effected by factors such as water composition and plumbing configuration, which will vary from house to house, as well as by consumer behaviour, which varies throughout the day.

1.2.3.1 Pipework configurations

The pipework configuration of a property will have a significant effect on the lead emissions that can be expected. To better understand the problem, a diagram of the pipework configuration used to supply drinking water for a typical property is shown (Figure 1.5). This illustrates the number of different combinations of plumbing materials that can be used in this standard configuration as well as indicating how the ownership of the plumbing is split between the water supplier and the consumer.

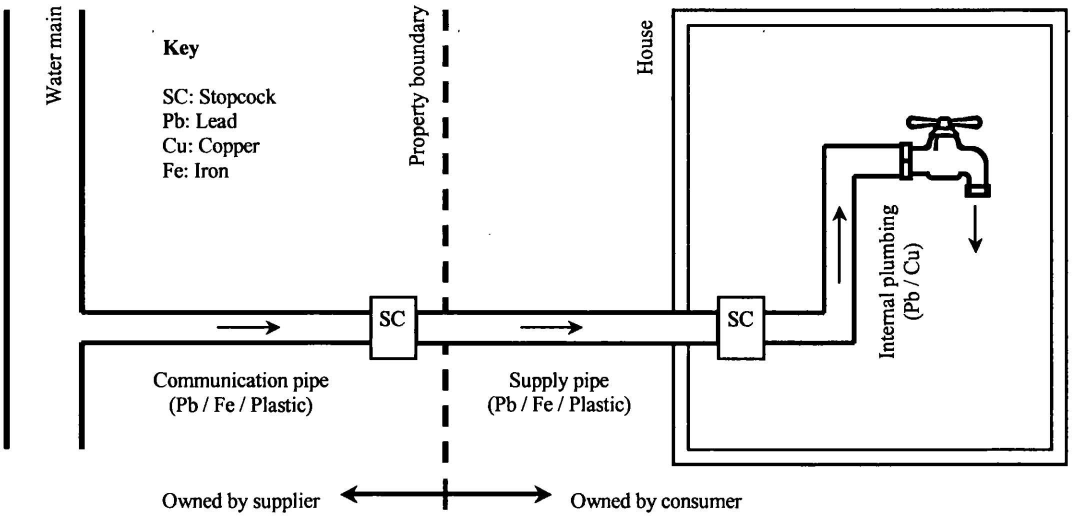


Figure 1.5. Typical pipework configuration at a property.

For simplicity, the term 'plumbing' will be used here to represent all the pipework that is used to transport the drinking water from the water main to the tap. It is a reasonable assumption that if a property has no lead plumbing, then it is unlikely to have any lead based solders or fittings. Thus, assuming lead salt stabilised uPVC is not used, the lead concentration of the drinking water at the tap, at any point during the day, will be zero. Note that the water supplied to the communication pipe by the water company has no lead content, since all water mains are now manufactured from non-lead materials.

However, lead emissions can be expected at a property if its drinking water is supplied through lead pipework, i.e. if any of the plumbing is made from lead, whether it is the communication pipe, service pipe or internal plumbing, or all of these. Approximately 40% of properties in the U.K. contain some length of lead pipework in their plumbing systems. In most cases this takes the form of the communication pipe or service pipe, which typically runs several feet underground from the road, where it connects to the water main, to the internal plumbing in the house, making it far harder to remove than the internal plumbing.

Lead emissions at properties are thought to increase with increasing lengths of lead pipework. This is because there is more surface area for the lead to dissolve into the drinking water from the pipe at any one time. It has also been shown that the diameter of the lead pipework can influence the dissolution of lead. Experimental results [50] suggest that the maximum lead concentration is reached after about 6 hours for pipes of 10mm internal diameter, whereas pipes of 50mm internal diameter take at least 50 hours.

1.2.3.2 Plumbosolvency

Plumbosolvency is a measure of the extent of dissolution of lead, i.e. the drinking waters ability to dissolve lead. As previously discussed, the plumbosolvency of lead in water depends on the composition of the water, particularly pH, alkalinity, ionic strength, organic content, and the redox potential, all of which determine the species of lead in solution and the solid that precipitates on the inner wall of the lead pipe. Thus, the lead emissions at a property will be highly dependant on the drinking water that is supplied, which, in turn, is dependant on geographical location, since chemical characteristics of drinking water vary considerably throughout the U.K.

Additionally, lead emissions are found to vary seasonally since plumbosolvency of a water is affected by temperature. As a general guide, lead concentrations tend to be about twice as high in the summer than in the winter. However, for waters having low plumbosolvency, the effect of temperature is less significant. Furthermore, in the case of water undergoing phosphate dosing, the trend reverses and lead emissions are found to decrease with increasing temperature (Figure 1.6) [60, 61].

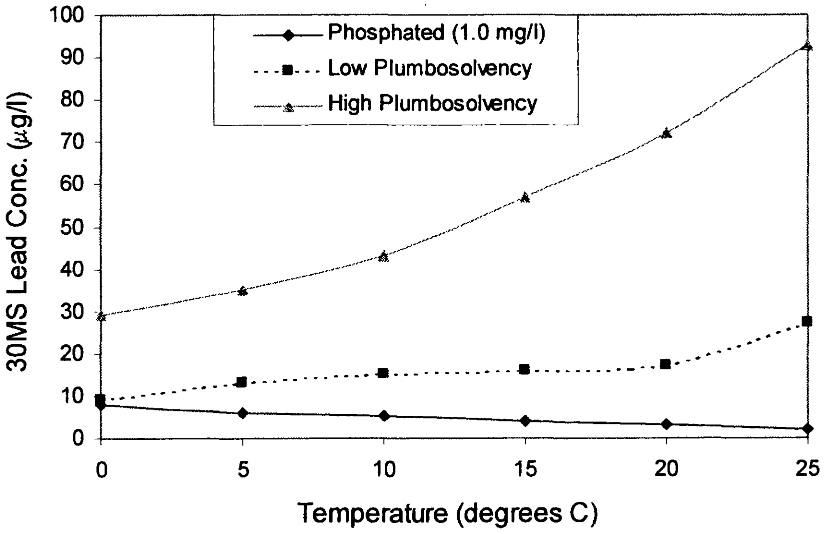


Figure 1.6. Variation of lead emissions with temperature.

The time – concentration response of water standing in a lead pipe accurately characterises the plumbosolvency of the water for that particular diameter lead pipe and is represented as a 'stagnation curve'. Figure 1.7 shows stagnation curves for three different waters, each having a different plumbosolvency.

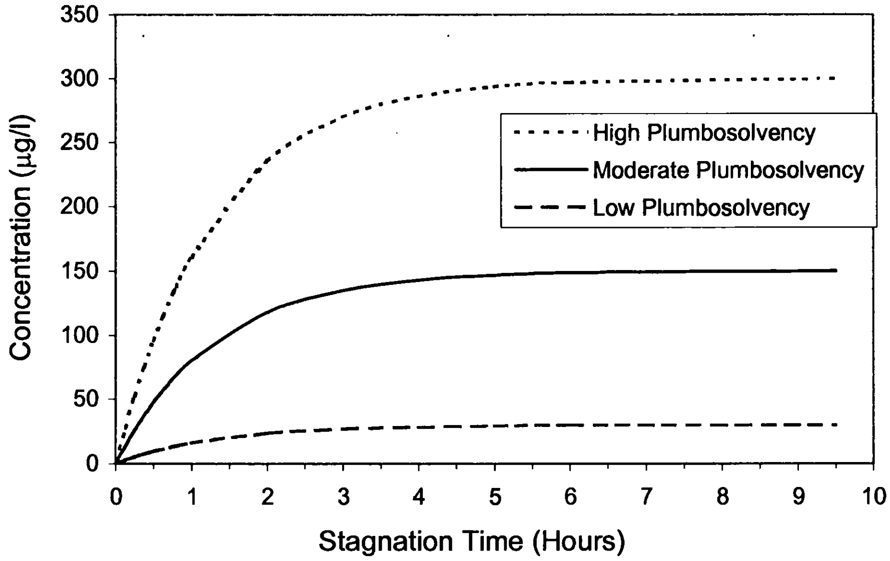


Figure 1.7. Stagnation curves for different waters.

For increasing plumbosolvency, it is clear that the lead concentration of drinking water standing in a lead pipe increases faster, i.e. the slope of the stagnation curve is steeper, and reaches a higher equilibrium concentration. This has a direct effect on lead emissions at a property, since for a given stagnation time, more lead is able to dissolve into the drinking water. Additionally, lead concentration in drinking water that has been standing in a lead pipe overnight will be higher.

1.2.3.3 Water usage

Consumer behaviour describes the manner in which the occupants of a household use water throughout the day, and has been found to influence the lead emissions at that property. The major influencing characteristics of water usage include the pattern of water usage, the volume of water used, and the flow rate. These can vary greatly from house to house, since they are influenced by the number of occupants and their lifestyle.

Studies have been carried out to measure the water usage characteristics for a range of different properties. Of these, Bailey et al. [62] conclude that, as expected, the number of persons in the household is the main factor influencing the consumption of water for non-potable purposes such as flushing of toilets and showering. However, the consumption of water for potable purposes appeared to be independent of household size. The mean inter-use time was found to be dependent on household size, the main difference being between single person, where inter-use time was greatest, and multi-person households [62]. There have been several attempts to characterise household water usage, namely the intensity, duration and frequency of water use, using mathematical models [63,64,65,66]. The chief motivation behind this work has been to predict residential water demand for the purposes of improving the design of water distribution systems. These models assume residential water demands occurs as a nonhomogeneous Poisson rectangular pulse process. Although this assumption is still inconclusive, the models developed have been found to be a reasonable approximation to actual water use.

The frequency of domestic water use varies considerably throughout the day in accordance with consumer lifestyle. The resulting pattern of water usage for a property is often skewed and reveals peak times during a day when water is very frequently used as well as extended periods of non-use, when the water is stagnant. Studies have shown that, on average, water use is diurnal, in that it is most frequently used in the morning before 11am and then again in the evening after 6pm, whilst water is rarely used between the hours of 1am and 6am. The water usage pattern can be characterised by a single quantity, namely the mean inter-use time. Whilst this has been shown [62] to decrease with increasing number of occupants, the average inter-use stagnation time has been found to be about 30 minutes. This value is in accordance with data observed in Germany, France and the Netherlands [22]. It should be noted that this average value of 30 minutes includes the overnight stagnation, which is usually about 6 hours; consequently, the mean inter-use time during the day is considerable shorter. Since lead concentration increases with stagnation time, in accordance with the stagnation curve, it is clear that longer inter-use times result in higher lead concentrations within the lead pipe immediately after the stagnation period. However, lead emissions in drinking water at the tap will also be effected by the volume of water drawn after the stagnation period.

The total volume of water used by the household during the day effects the contact time of the water with plumbing materials, and as a result the quantity of lead that dissolves into the water. Thus, when a household uses larger volumes of water, the average lead concentration of drinking water at the end of the day will reduce since this larger volume of water effectively dilutes the lead that dissolves. However, although the concentration of lead in the water reduces, the actual daily quantity of lead ingested from the drinking water may not reduce if proportionally larger quantities of drinking water are ingested.

It is not clearly understood how the flow rate effects lead emissions; however, research [22,67] has shown that lead concentration is higher when the flow in the pipes is turbulent as opposed to laminar, i.e. when the flow is fast as opposed to slow. This may be caused by the release of particulate lead since turbulent flow causes higher shear stresses on the pipe wall, which may cause flaking of fragile lead corrosion products from the inside wall of the lead pipe. In practice, consumers draw water with an average flow rate of approximately 5 litres/minute, which corresponds to turbulent flow for most pipework [22].

1.2.4 Water supply zones

The responsibility for providing drinking water in England and Wales rests with private water companies. Around 25% of the population in England and Wales is provided with drinking water by smaller private water companies, whilst the majority of water users are customers of the 10 privatised water companies, these include Anglian Water Services Limited and North West Water Limited. The region served by the water company is broken up further into more manageable areas called water supply zones.

Water supply zones are the spatial designation relevant to serviceability measures and the principal unit for regulatory and technical decision making within the UK and other European countries. Water companies define water supply zone boundaries and are permitted to change the delineation every year. The current limit on zone size is 50,000 population but this is due to change to 100,000 in 2004. The current average zone size in the U.K. is in the region of 20,000 population. At present zones are usually defined on practicable bases that include a requirement for hydraulic separation [68]. A water supply zone typically encompasses a rural or urban district, such as a village or small town. Since the current limit on zone size is 50,000 larger towns and cities are broken up into a number of water supply zones.

1.2.4.1 Typical configurations

The average water supply zone in the U.K. has a population of approximately 20,000 consumers and, on average, approximately 40% of these are supplied through lead pipework. However, the proportion of properties supplied through lead pipework is highly dependant on geographical location and newer city districts are likely to have considerably less lead pipework than older districts.

Since housing characteristics, such as age and size, can vary considerably across a zone, it is clear that the design, dimensions, and materials used in plumbing systems will also vary. Surveys have shown that in some isolated situations, the lead pipework used to supply a property can be as long as 70 – 100m; though in most cases it has been found to be fairly short, of the order of 5 – 20m. Non-lead pipework is also likely to be present at properties that have lead pipework since the internal lead plumbing is often replaced using a non-lead material, usually copper. This is also likely to vary in length across the water supply zone due to the diversity of plumbing installations. Virtually all of the internal domestic plumbing in the U.K. has been found to be of 12mm internal diameter pipework, though the communication pipe may vary in diameter to a small extent.

As well as plumbing circumstances, consumer behaviour is likely to vary significantly across a water supply zone. Thus, the quantity of water used throughout a day and the pattern and frequency with which the water is used, will vary across the zone. As previously discussed, consumer behaviour at a property is influenced by the number of occupants and their lifestyle; it is not usually influenced by the plumbing circumstances. Thus, it is possible to have a property that has considerable lead pipework and the occupant(s) use very little water.

For most water supply zones, particularly where the water being supplied is of high alkalinity, the quality of water throughout the zone is fairly uniform; consequently the plumbosolvency of the water does not vary appreciably. However, some zones suffer distinct changes in water quality that affect plumbosolvency, as is the case for many low alkalinity waters which suffer a pH reduction as the water passes through the distribution system. This has the effect of increasing the plumbosolvency of the water at the extremities of the water supply zone, where the distance from the waterworks is greatest. There is also the possibility that outlying regions of a zone can be supplied by water from two separate waterworks, thus the water actually supplied will be a mixture having different chemical properties, and therefore a different plumbosolvency from the water that is supplied to the rest of the water supply zone.

It is not logistically practical to develop a completely accurate description of a water supply zone in terms of pipework configurations, consumer behaviour and water quality variation. Thus, these characteristics must be estimated from data obtained through limited surveys and investigations.

1.2.4.2 Shared communication pipes

In most water supply zones in the U.K. the housing is almost exclusively detached, semi-detached or terraced. In these cases the properties are supplied with drinking water from the water main via a single communication pipe as depicted in Figure 1.5. However, water supply zones in cities or at the centre of large towns are likely to contain a significant proportion of properties in the form of high-rise flats or apartment blocks. Such properties will usually be supplied with drinking water via a shared communication pipe as depicted in Figure 1.8. The number of properties supplied through each communication pipe may vary considerably.

The water usage of one property can effect the lead emissions at another if they both share the same lead communication pipe. For example, if the first property that used water in the morning, was to run the tap for long enough, then the drinking water that had stagnated in the shared communication pipe overnight would be supplied to that property. As this lead-rich water was drawn through the shared communication pipe, it would be replaced by fresh water from the water main. Consequently, when the neighbouring property uses water after the first property, the lead concentration of the water in the shared communication pipe will be considerably less than it would have been had the neighbour not used water before them.

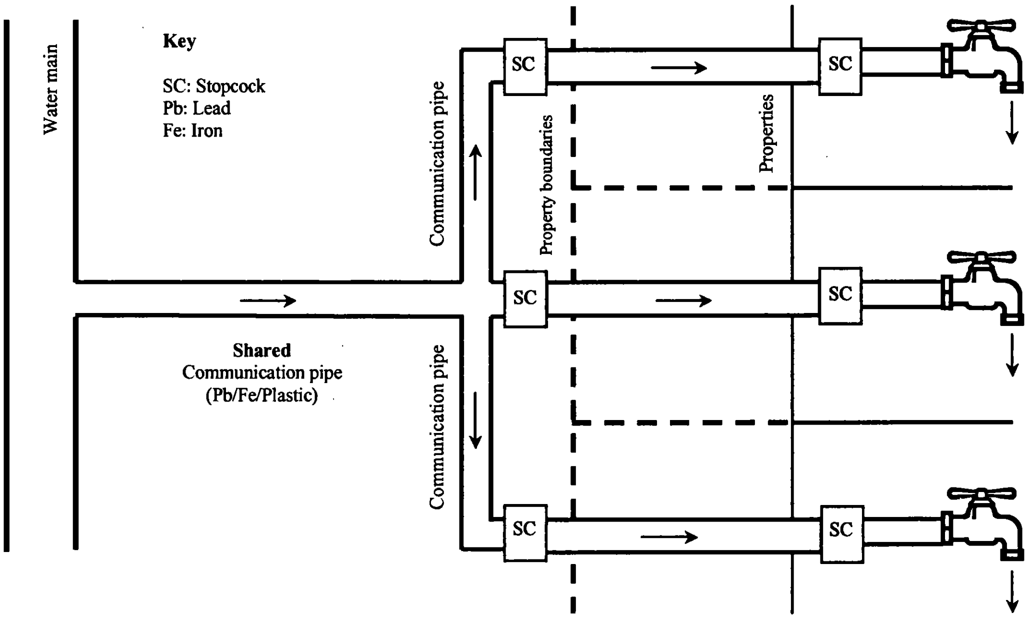


Figure 1.8. Shared communication pipes.

1.2.5 Assessing zonal compliance

1.2.5.1 Daily average concentration

The new "drinking water" directive indicates that the limits of 10μg/l and 25μg/l must be related to the weekly average concentration at individual properties. Thus, in order to assess the exact compliance with the new lead standards, it would be necessary for the water supplier to measure the lead emissions at the tap during one week, every time the tap is turned on, for every single consumer in each water supply zone they serve. Although this method would provide the most accurate assessment possible, it is clearly not a practical option in real life. However, daily and weekly average lead emissions at a small number of properties in the water supply zone can feasibly be measured accurately by the composite proportional (COMP) sampling method previously discussed. An outline of the basic processes involved in this procedure is as follows:

- ❖ For every house in the COMP sampling survey:
  - Randomly select house from water supply zone.
    - o Over the course of one day or one week:
      - ▪ For every time water is used from kitchen tap:
        - ➢ Divert 5% of it into the sample bottle.

    - Measure concentration of lead in sample bottle at the lab.
- Calculate compliance of zone based on failure rate of sample concentrations against 10 and 25μg/l standard.

This technique is reproducible and representative for a single property, however, since lead emissions vary widely throughout most water supply zones, due to differences in plumbing and consumer behaviour, this technique does not often represent zonal compliance well because the number of samples that can realistically be taken using this method is so low.

1.2.5.2 RDT sampling

The most widely used sampling technique, employed by water suppliers in the UK, is Random Day Time (RDT) sampling. This approach has been used extensively for assessing compliance with lead standards since 1989 and remains the most favoured protocol in terms of costs, practicality and consumer acceptance. An outline of the basic processes involved in this procedure is as follows:

- For every house in the RDT sampling survey:
  - Randomly select house from water supply zone.
    - Pick a random time during the day (9am-5pm) to access house.
    - If access is not possible:
      - House next door is tried, and so on, until access is gained.
    - If access is possible:
      - Take one-litre sample from the kitchen cold-water tap without prior flushing.
    - Measure concentration of lead in sample bottle at the lab.
- Calculate compliance of zone based on failure rate of sample concentrations against 10 and 25μg/l standard.

As opposed to COMP sampling, this procedure is not reproducible at a single property because lead emissions at an individual property vary throughout the day, and the RDT sample result for a property is merely a measure of lead emissions at one instant during the day. This problem compounds across a water supply zone due to the wide variability in factors that effect lead emissions; a problem inherent in sampling. It should be noted however that many more samples can be taken for RDT sampling than for COMP sampling since it is much more cost effective and practical. Consequently, in general, assessment of zonal compliance is likely to be more reproducible when using RDT sampling due to the considerably higher sample size possible.

2 SINGLE HOUSE

2.1 Lead system in a single house

2.1.1 Geometry and co-ordinates of pipe system

In order to accurately describe the physical processes taking place within a simple pipework system, it is first necessary to set up a domain and co-ordinate system for the problem. The most basic element of a pipework system is a single length of straight pipe having circular cross-section with an internal radius of r_0. The physical processes of fluid flow and mass transfer take place within the water enclosed by the pipe, i.e. within the cylindrical domain that is bounded by the inner pipe wall. Since the pipe is symmetric it is intuitive to set up a 3-D cylindrical polar co-ordinate system as shown (Figure 2.1), where x, r, and θ denote the longitudinal, radial, and angular co-ordinate axis respectively.

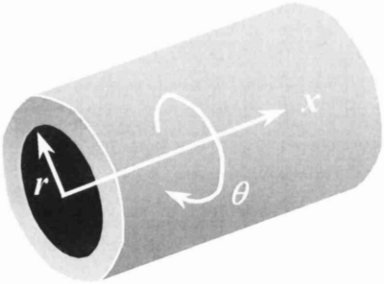


Figure 2.1. Co-ordinate system of a pipe.

It will be necessary to model the movement of the water within the domain that has been defined. Thus, the principal fluid velocity components are denoted by u (velocity in the x-direction), v (velocity in the r-direction) and w (velocity in the θ-direction).

2.1.2 Mass Transfer

The transfer of the lead from the wall of the lead pipe into the water, and the transfer of dissolved lead along the pipe when the water is flowing, must be modelled in order to simulate lead emissions at the tap. Thus, it is necessary to formulate or obtain an accurate mathematical description of the mass transfer processes that take place within a water filled pipe.

2.1.2.1 Conservation of mass

Consider first an illustration of the system (Figure 2.2) showing the basic processes taking place when the water is: (a) stationary; (b) flowing at an arbitrary volumetric flow rate Q through the pipe.

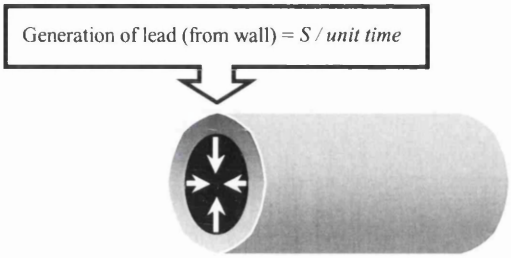


Figure 2.2a. Mass transfer in a section of lead pipe when water is stationary.

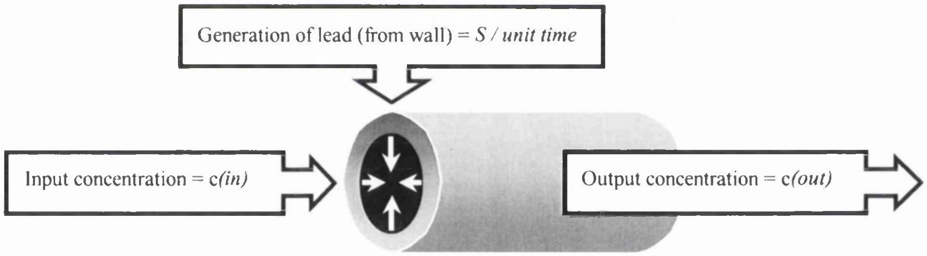


Figure 2.2b. Mass transfer in a section of lead pipe when water is flowing.

When the water is stationary, the only process taking place is the generation of lead in the water through the dissolution of lead from the internal surface of the pipe. However, when the water is flowing additional processes take place, namely the input of lead into the system and the output of lead from the system.

The conservation of mass must be applied to this system. This is the fundamental principle that states 'mass cannot be created or destroyed but it may change form' and in the case of dissolved lead in a pipe may be expressed as:

(Accumulation of lead / unit time) = (Flow of lead into pipe / unit time) – (Flow of lead out of pipe / unit time) + (Generation of lead in the pipe / unit time) Eqn. 2.1

This may be re-written in terms of concentration of lead, and flow rate as:

$$\frac{\partial c}{\partial t}V = Qc(in) - Qc(out) + S \qquad \text{Eqn. 2.2}$$

where *c, V* and *S* are the concentration of lead, generation of lead per unit time and volume of the section of pipe respectively. Dividing by *V* and then substituting $u/\Delta x = Q/V$ gives:

$$\frac{\partial c}{\partial t} = u\left[\frac{c(in) - c(out)}{\Delta x}\right] + \frac{S}{V} \qquad \text{Eqn. 2.3}$$

where Δx is the length of the section of pipe and *u* is the velocity of the water in the *x*-direction, i.e. along the length of the pipe. Finally, substituting:
$\partial c/\partial x = [c(out) - c(in)]/\Delta x$ gives:

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} + \frac{S}{V} \qquad \text{Eqn. 2.4}$$

2.1.2.2 Fick's law of diffusion

Diffusion is the mechanism by which components of a mixture, e.g. dissolved lead, are transported around the mixture by means of random molecular (Brownian) motion. The flow of mass per unit area by diffusion (i.e. the Flux) across a plane, is proportional to the negative concentration gradient of the diffusant across that plane [69]. This states that mass will move from positions of high concentration to positions of low concentration (i.e. move in the direction of a negative concentration gradient). This is Fick's First Law, and in an arbitrary direction *Z* can be expressed as:

$$Flux = -D\frac{\partial c}{\partial Z} \qquad \text{Eqn. 2.5}$$

where *D* is the coefficient of diffusion.

If there are more atoms of lead entering a small volume than there are leaving it, the concentration will increase with time, and visa versa. We can express this idea in mathematical notation as follows: $\partial Flux/\partial Z = -\,\partial c/\partial t$, where t is time. Fick's Second Law is then derived by taking a partial derivative of both sides of Eqn. 2.5 with respect to Z, giving:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial Z^2} \qquad \text{Eqn. 2.6}$$

In terms of a radial coordinate system in the r-direction this becomes:

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r}\right) \qquad \text{Eqn. 2.7}$$

2.1.2.3 Mass transfer in three dimensions

A full mathematical description of mass transfer within a section of pipe can now be obtained by incorporating the principal of conservation of mass and Fick's laws to the system. The generation of lead within the pipe is through the diffusion of lead from the inner wall of the lead pipe into the water; hence the *S/V* term in Eqn. 2.4 can effectively be replaced by the right-hand-side of Eqn. 2.7. Allowing for flow and diffusion in all directions, this mass transfer equation then becomes:

$$\frac{\partial c}{\partial t} = \underbrace{-\left(u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial r} + w\frac{\partial c}{\partial \theta}\right)}_{Advection} + \underbrace{D\left[\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r} + \frac{1}{r^2}\frac{\partial^2 c}{\partial \theta^2}\right]}_{Diffusion} \qquad \text{Eqn. 2.8}$$

The full mass transfer equation in three dimensions (Eqn. 2.8) describes how the concentration c, of a substance within the water inside the pipe, varies spatially and temporally, with respect to the principal velocities of the fluid (u, v, w) and the coefficient of diffusion D (m^2/s). Note that the equation has been written in cylindrical polar co-ordinates, as this is most appropriate for modelling mass transfer in a cylindrical domain, i.e. a pipe.

Lead enters the water at the inner wall of the lead pipe through a process of diffusion (particulate lead will be ignored). When the water is flowing, the lead that has entered the water will travel along the length of the pipe, being carried by the movement of the water. This is known as advection. Note that diffusion of lead from the inner wall of the lead pipe into the water will also occur during flow.

2.1.3 Flow in a pipe

2.1.3.1 Navier-Stokes equations

To accurately model a real fluid, it is necessary to take into account its density and its viscosity. Consider an incompressible flow of a real fluid, such as water, through a pipe having the cylindrical polar co-ordinate system (x, r, θ) with the corresponding principal velocity components (u, v, w) as described previously. It can be shown [70,71] that the continuity equation (principal of conservation of mass of the fluid itself) may be expressed as:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial u\rho}{\partial x} - \frac{\partial v\rho}{\partial r} - \frac{1}{r}\frac{\partial w\rho}{\partial \theta} \qquad \text{Eqn. 2.9}$$

where ρ is density. When density is constant this becomes:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial r} + \frac{1}{r}\frac{\partial w}{\partial \theta} = 0 \qquad \text{Eqn. 2.10}$$

The law of conservation of momentum states that a body or volume of fluid in motion cannot gain or lose momentum unless some external force is applied. These external forces may include pressure, shear stress and 'body forces' such as gravity. Application of the principal of conservation of momentum to an incompressible flow in three dimensions yields the following relationships:

$$\begin{aligned}
\rho\frac{\partial u}{\partial t} &= -\rho\left\{u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial r} + \frac{w}{r}\frac{\partial u}{\partial \theta}\right\} + \mu\left\{\frac{\partial^2 u}{\partial x^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2}\right\} - \frac{\partial p}{\partial x} + \rho g_x \\
\rho\frac{\partial v}{\partial t} &= -\rho\left\{\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial r} + \frac{w}{r}\frac{\partial v}{\partial \theta} - \frac{w^2}{r}\right\} + \mu\left\{\frac{\partial^2 v}{\partial x^2} + \frac{1}{r}\frac{\partial v}{\partial r} + \frac{\partial^2 v}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 v}{\partial \theta^2} - \frac{2}{r^2}\frac{\partial w}{\partial \theta}\right\} - \frac{\partial p}{\partial r} + \rho g_r \qquad \text{Eqn. 2.11} \\
\rho\frac{\partial w}{\partial t} &= -\rho\left\{\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial r} + \frac{w}{r}\frac{\partial w}{\partial \theta} + \frac{vw}{r}\right\} + \mu\left\{\frac{\partial^2 w}{\partial x^2} + \frac{1}{r}\frac{\partial w}{\partial r} + \frac{\partial^2 w}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 w}{\partial \theta^2} + \frac{2}{r^2}\frac{\partial v}{\partial \theta}\right\} - \frac{\partial p}{\partial \theta} + \rho g_\theta
\end{aligned}$$

where μ is the viscosity of the fluid, g is the gravitational force acting on the fluid, and p is the pressure of the fluid [71].

These are the Navier-Stokes equations. They are written in cylindrical co-ordinate form, as this is most appropriate for the problem that is being dealt with. The complete derivation of these equations has not been included as it is fairly lengthy. In essence, these equations describe how the velocity of the fluid changes temporally and spatially.

2.1.3.2 Laminar flow

Flow in pipes can be categorised into three distinct patterns; they are laminar flow, transitional flow and turbulent flow. Laminar flow typically occurs at relatively low velocities; here the fluid may be considered to flow in discrete layers with no mixing. In transitional flow there is some degree of unsteadiness. Finally in turbulent flow the fluid incorporates an eddying or mixing action [70].

The governing equations of laminar flow may be derived from the Navier-Stokes equations by making some simple assumptions. For simplicity, it is assumed that the fluid is only flowing in the x-direction, i.e. along the length of the pipe. Thus, there is no velocity in the radial or angular directions, r and θ, i.e. $v = 0$ and $w = 0$. It is also necessary to assume that the flow is steady, i.e. there is no variation in velocity over time. This particular assumption is completely accurate only if the fluid is continuously flowing through the pipe. This is not the case in the problem we are trying to model; however, it does greatly simplify the problem. The flow is also assumed to be uniform, i.e. the velocity is constant along the whole length of the pipe. Finally we must assume that there are no body forces acting on the fluid.

Making these assumptions enables the Navier-Stokes equations (Eqn. 2.11) to be simplified considerably to:

$$\frac{\partial p}{\partial x} = \mu\left[\frac{1}{r}\frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial r^2}\right] \qquad \text{Eqn. 2.12}$$

We now have an equation relating pressure gradient, radius of pipe and velocity of fluid. By integrating we may solve for u to give:

$$u = \frac{1}{4\mu}\frac{dp}{dx}r^2 + c_1 \log r + c_2 \qquad \text{Eqn. 2.13}$$

In order to determine the two constants of integration the following boundary conditions are applied: $u = 0$ at $r = r_0$ and $u =$ finite at $r = 0$, where r_0 is the radius of the pipe. The first is the 'no slip' boundary condition, principal to viscous fluids, which ensures the fluid 'sticks' to the pipe wall as opposed to 'sliding' along it. Substituting these boundary conditions into Eqn. 2.13 gives:

$$u = -\frac{1}{4\mu}\frac{dp}{dx}\left(r_0^2 - r^2\right) \qquad \text{Eqn. 2.14}$$

The discharge or volumetric flow rate Q may be determined by integrating through all the annuli that make up the cross-section of the pipe:

$$Q = 2\pi \int_{0}^{r_0} urdr \qquad \text{Eqn. 2.15}$$

Substituting the expression for u from Eqn. 2.14 into Eqn. 2.15 and integrating gives:

$$Q = -\frac{\pi}{8\mu}\frac{dp}{dx}r_0^4 \qquad \text{Eqn. 2.16}$$

This is then rearranged and substituted into Eqn. 2.14 to give:

$$u = \frac{2Q}{\pi r_0^4}\left(r_0^2 - r^2\right) \qquad \text{Eqn. 2.17}$$

Thus, from Eqn. 2.17 it is clear that given a constant flow rate, the velocity of the fluid decreases with r, i.e. the distance from the centre of the pipe, from a maximum in the centre of the pipe to zero at the pipe wall where the no-slip boundary condition has been imposed. This relationship is depicted in Figure 2.3. Note also that the maximum velocity is exactly double the average velocity.

2.1.3.3 Turbulent flow

The motion of fluid particles within a turbulent flow is complex and irregular, involving fluctuations in velocity and direction making it very hard to model realistically with mathematics. Due to it's stochastic nature it is often necessary to resort to statistical techniques as a solution method. Since the velocity varies continuously with time, it may be broken down into time averaged and fluctuating components for simplicity. Thus the velocity in the x-direction becomes $u + u'$ etc. Applying this concept throughout leads on to the Navier-Stokes equations for turbulent flow. These describe the fluid movement well but simple solutions cannot be obtained [70].

The simplest and most effective way of modelling turbulent flow is to use experimental data. It is known from experiment that the time averaged velocity profile for turbulent flow in a pipe is fairly flat, except in the vicinity of the wall. For many purposes a simple power law is a good approximation. The most widely used power law is the One-Seventh-Power Law [70]:

$$\frac{u}{u_{\max}} = \left(\frac{r_0 - r}{r_0} \right)^{1/7} \qquad \text{Eqn. 2.18}$$

Eqn. 2.18 simply relates the velocity at any position r to the maximum velocity, which occurs in the centre of the pipe as in laminar flow. It can be readily shown that the average velocity is directly related to the maximum velocity as follows:

$$\bar{u} = 0.817 \times u_{\max} \qquad \text{Eqn. 2.19}$$

However, average velocity may also be found using:

$$\bar{u} = \frac{Q}{A} = \frac{Q}{\pi r_0^2} \qquad \text{Eqn. 2.20}$$

By substitution we obtain:

$$u_{\max} = \frac{Q}{0.817 \pi r_0^2} \qquad \text{Eqn. 2.21}$$

Finally, this expression for u_{max} is substituted into Eqn. 2.18 to give:

$$u = \frac{Q}{0.817 \pi r_0^2} \left(\frac{r_0 - r}{r_0} \right)^{1/7} \qquad \text{Eqn. 2.22}$$

Once again, from Eqn. 2.22 it is clear that given a constant flow rate, the velocity of the fluid varies with the distance from the edge of the pipe. This relationship is depicted in Figure 2.3.

2.1.3.4 Inviscid (plug) flow

The above expressions that describe laminar and turbulent flow have been derived by assuming the water has viscosity. However, fluid flow through a pipe can be modelled in varying levels of complexity; the simplest method is to assume that the fluid has no viscosity, i.e. it is inviscid. In this case, the velocity of the fluid u is constant across the cross-section of the pipe and is readily calculated as Q/A. This is known as inviscid (or plug) flow. Figure 2.3 illustrates how plug flow approximates well to turbulent flow across most of the pipe's cross-section except in the vicinity close to the pipe wall.

However, the wall effects are much greater in laminar flow, consequently plug flow does not approximate well in this case.

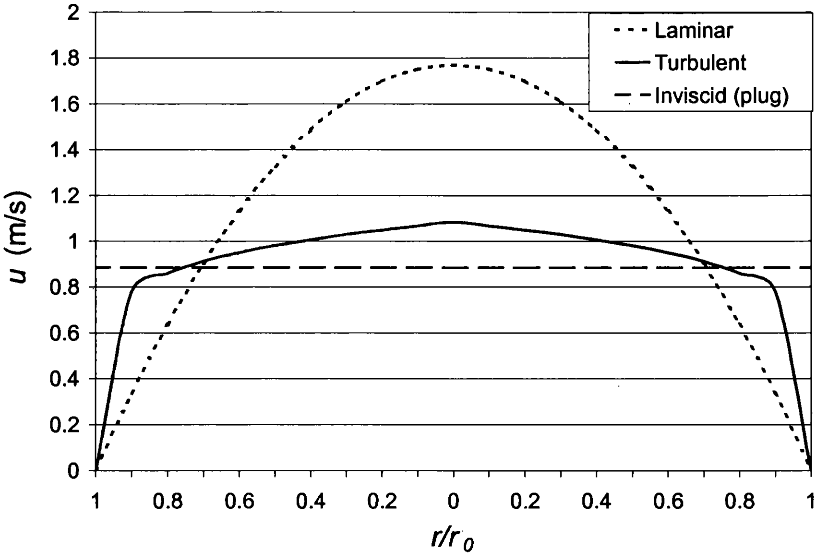


Figure 2.3. Fully developed velocity profile of laminar, turbulent and inviscid flow.

2.1.3.5 Reynolds number

Reynolds' experiments revealed that the onset of turbulence was a function of fluid velocity, viscosity and a typical dimension. This led to the formulation of the dimensionless Reynolds Number Re, which represents the ratio of inertial force to viscous force in a fluid [70]. It is possible to predict whether the flow in a pipe is laminar or turbulent by calculating the Reynolds number. For a fluid moving with average velocity $\bar{u}$ through a pipe of radius r_0 it can be shown that:

$$Re = 2r_0\rho\bar{u}/\mu \qquad \text{Eqn. 2.23}$$

Having determined the Reynolds number it is a simple matter of comparing this figure to other values corresponding to known types of flow. For example, flows in pipes normally conform to the following pattern:

- $Re < 2000$: Laminar flow
- $2000 < Re < 4000$: Transitional flow
- $Re > 4000$: Turbulent flow

However, these values should only be used as a rough guide as some experiments have revealed laminar flows occurring for $Re >> 4000$ [70]. However, even as a rough guide, this enables one to use the most appropriate velocity profile by performing one simple calculation.

2.1.3.6 Shear stresses on the pipe

A viscous fluid is able to transmit a shear stress. This shear stress is proportional to the rate of change of velocity across the cross-section of the pipe (Eqn. 2.24).

$$\tau = constant \times \frac{du}{dr} \qquad \text{Eqn. 2.24}$$

For a typical velocity profile within a straight section of pipe, shear stress can be plotted across the cross-section of the pipe (Figure 2.4). Note that the shear stress increases linearly from zero in the centre of the pipe to a maximum of τ_0 on the inner wall of the pipe. For fluid flowing through a curved pipe or bend, the shear stress on the outside of the bend increases further since it is due to both viscosity and inertial components. It is thought that high shear stress on the inner pipe wall could be responsible for dislodging flakes of corrosion deposit and contribute to particulate lead. However, at present this phenomenon has not been quantified.

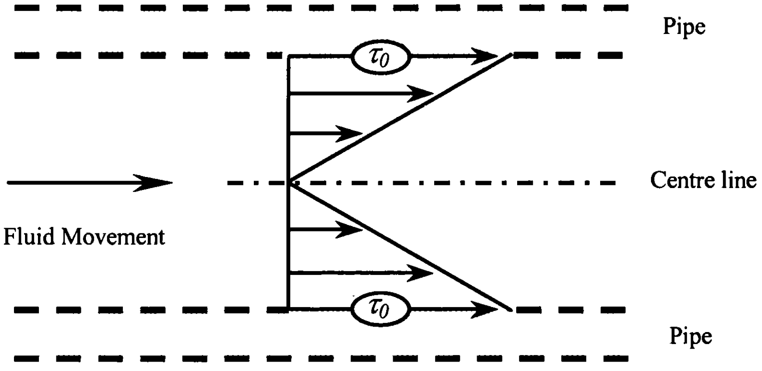


Figure 2.4. Shear stresses in a straight pipe.

For laminar flow in a straight pipe, it can be shown that:

$$\tau = 4\mu\bar{u}r/r_0^2 \qquad \text{Eqn. 2.25}$$

hence, the shear stress at the pipe wall, τ_0 is readily found:

$$\tau_0 = 4\mu\bar{u}/r_0 \qquad \text{Eqn. 2.26}$$

However, for turbulent flow in a straight pipe, the shear stresses are larger and have to be calculated using semi-empirical formulae:

$$\tau_0 = \frac{\lambda \bar{u}^2 \rho}{8} \qquad \text{Eqn. 2.27}$$

where, λ must be calculated using Moody and Barr formulae [70].

2.2 Modelling a single house

2.2.1 Modelling pipework

2.2.1.1 Physical description

As previously discussed, lead emissions in drinking water are effected by factors such as water composition, plumbing configuration and consumer behaviour. In order to model the transfer of lead from the lead pipework to the water drawn through the tap, it is first necessary to define the physical geometry of the pipework. Plumbing configurations at a single property can often be complex, containing many branches and bends in the pipes. Additionally, a variety of plumbing materials may be used at a single property. However, since lead emissions at the kitchen tap are to be modelled, the only physical portion of the plumbing system that needs to be represented is the pipework between the water mains and the kitchen tap.

In general, properties are unlikely to have lead pipes being used in the internal plumbing since these are usually replaced with a non-lead alternative. Thus, where a property contains lead pipework, it is usually in the form of the supply pipe and communication pipe that runs underground between the water main and the property [61]. Consequently, for any property containing lead plumbing, it is assumed that the pipework connecting the water main to the tap can be represented by a length of lead pipe coupled to a length of non-lead pipe (Figure 2.5). Since copper is the most popular 'non-lead' material for plumbing, the 'non-lead' pipe will usually be referred to as the copper pipe.

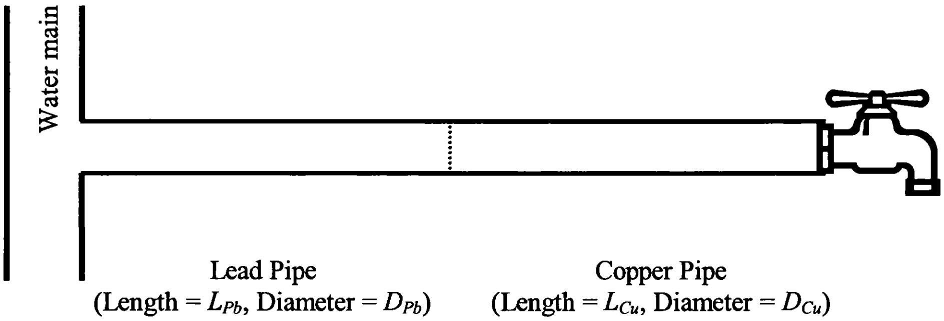


Figure 2.5. Representation of pipework.

The geometry of the domain is thus described by the dimensions of the lead pipe and the copper pipe; the lengths of which vary considerably across water supply zones.

However, in the UK, the internal diameter of pipework between the water mains and the tap is generally found to be 12mm [61].

2.2.1.2 Assumptions

It is often necessary to make a number of assumptions before a process can be modelled. Assumptions usually consist of a set of rules or conditions that are imposed in order to simplify the process sufficiently for a model to be developed. Consequently, it will be necessary to make a number of assumptions to simplify the complex processes taking place within the pipework, since a primary objective of this research was to develop a computational model that can run on modest computing resources. Furthermore, there is little point modelling the physical processes in great detail if basic parameters, such as length of pipework and daily water consumption, are not accurately known.

A key assumption has already been made in order to characterise the pipework configuration, namely that the pipework connecting the water main to the tap can be represented by a length of lead pipe coupled to a length of non-lead pipe (Figure 2.5). Additionally, for simplicity it is assumed that the pipework connecting the water mains to the tap is perfectly straight, although in reality there may be a number of bends in the pipework. The justification for this is to facilitate the modelling of otherwise highly complex fluid and mass transfer processes whilst keeping enough detail to allow for an accurate representation of the situation.

Assumptions concerning flow characteristics are required in order for the laminar and turbulent flow equations (Eqn. 2.17 and Eqn. 2.22) previously derived, to be used to model the movement of the fluid within the pipe. These assumptions are as follows:

- Flow has axial symmetry, i.e. no velocity variation in the θ-direction. This is a reasonable assumption considering a perfectly straight pipe of circular cross-section is also symmetric in the θ-direction.

- Flow is steady, i.e. there is no variation in the velocity profile over time. This particular assumption is completely accurate only if the fluid is continuously flowing through the pipe, implying that the tap is either fully open or fully closed. In this case the fluid's acceleration from rest to full flow is not modelled.

- Flow is fully developed or uniform, i.e. there is no variation in the velocity profile along the length of the pipe. In reality, boundary layer growth occurs at the entry to the pipe causing the velocity profile to stretch, this continues downstream until the flow becomes fully developed. Generally this occurs approximately *50D* downstream for turbulent flow and *110D* downstream for laminar flow, where *D* is the internal diameter of the pipe [70]. This equates to 0.6m for turbulent flow and 1.3m for laminar flow, assuming pipework of 12mm internal diameter, which is insignificant compared to the total length of pipework at a typical property.

- There are no body forces acting on the fluid.

These assumptions also hold for plug flow, though this flow also assumes that the fluid has zero viscosity.

2.2.1.3 Discretisation of pipework

In order to model how the concentration of lead within the water varies spatially, it is necessary to discretise the domain, i.e. the pipework, along the axis (i, $i = 1, N$), and in the radial direction (j, $j = 1, J$) as illustrated (Figure 2.6). Additionally, Δx is the increment in the axial direction ($\Delta x = L/N$), where L is the length of pipe, and Δr is the increment in the radial direction ($\Delta r = r_o/J$).

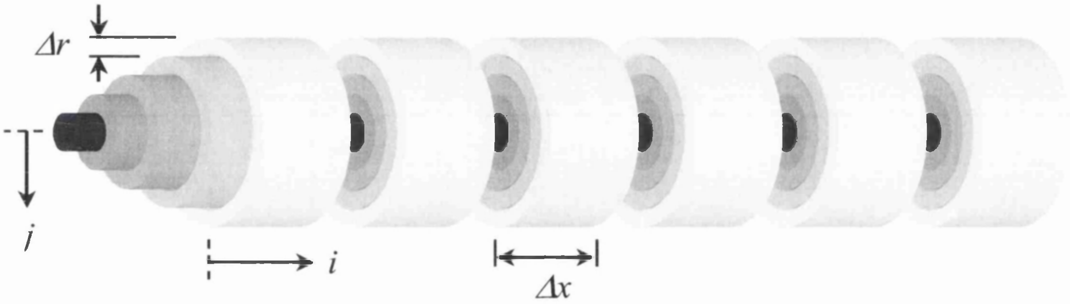


Figure 2.6. Discretisation of pipework.

In order to model temporal variation of lead in water, e.g. when water is flowing through the pipework; it is necessary to discretise the time (t, $t = 1,n$) for which the 'flow time' or 'stagnation time', of length T, takes place. Thus, similarly to the spatial discretisation described, Δt is the increment in time ($\Delta t = T/n$).

The number of axial elements N is dependant on the length of the pipe L and the timestep Δt. It is necessary to impose the condition that the volume of water in any axial element cannot be completely emptied in less than one timestep. The implications of this would be that the model would not function properly as it would effectively be predicting concentrations. This condition may be written as:

$$u_{\max}\Delta t \le \Delta x \qquad \text{Eqn. 2.28}$$

As discussed previously, the maximum velocity of fluid within a pipe u_{max} occurs in the centre of the flow. Since plug-flow assumes a uniform velocity profile, the maximum velocity u_{max} is simply found from the flow rate and internal cross-sectional area of the pipe:

$$u_{\max} = u = Q/\pi r_0^2 \qquad \text{Eqn. 2.29}$$

For laminar flow it is known that:

$$u_{\max} = 2Q/\pi r_0^2 \qquad \text{Eqn. 2.30}$$

Similarly for turbulent flow, it is known that:

$$u_{\max} = Q/0.817\pi r_0^2 \qquad \text{Eqn. 2.31}$$

For a timestep of $\Delta t = 1\ sec$ and a flow rate of $Q = 0.0001\ m^3/s$ ($0.1\ l/s$), the minimum axial increment Δx is found to be *0.88m*, *1.77m* and *1.08m* for plug-flow, laminar flow and turbulent flow, respectively.

However, for pipework lengths smaller than this, the timestep must be reduced in accordance with the second condition that must be imposed, namely $N \geq 1$. This states that the pipe must contain at least one axial element; the allowable timestep can then be obtained by substituting $L \geq \Delta x$ into Eqn. 2.28 to give:

$$\Delta t \leq L/u_{\max} \qquad \text{Eqn. 2.32}$$

2.2.2 Modelling water usage

In addition to the pipework characteristics, a major contributing factor to household lead emissions is consumer behaviour, i.e. the way in which the water is used during the day. Consequently, if lead emissions are to be modelled over the course of an entire day, it is necessary to specify exactly how the water is to be used throughout the entire day. The characteristics of water usage that need to be specified are the pattern of water usage, the total daily volume of water used, and the flow rate.

The flow rate Q will determine whether the flow in the pipework is laminar or turbulent. Generally, in domestic situations, water is drawn through the kitchen tap at about *0.1 l/s*

(0.0001m³/s). Assuming the internal diameter of the domestic pipework is *12mm*, then from Eqn. 2.23 the Reynolds number is found to be approximately *9000*, which indicates that the flow is likely to be turbulent. For simplicity it is assumed that the flow rate is the same each time the tap is turned on, though in reality it will vary to some extent.

The total daily volume of water used, V^T *(m³)*, is defined for a single house. This will determine the total flow time F^T *(sec)*, i.e. the total time during the day for which water is being drawn from the tap. For a given flow rate Q *(m³/sec)*, it is clear that

$$F^T = V^T / Q \qquad \text{Eqn. 2.33}$$

Clearly, the total volume of water V^T is used throughout the day, in varying quantities, rather than all at once. Consequently, to model specific water usage throughout the day, it is necessary to split the 24-hour day into discrete time periods. This will allow the application of a 'pattern of water usage', which describes how much water is used during each discrete time period.

An example of such a pattern (Figure 2.7) illustrates how domestic water demand varies throughout the day. Generally, peak water usage occurs between *7am* and *8am* when people are using showers and toilets shortly after waking up. A subsequent peak may occur during lunchtime if people are home at this time, as is the case in this example. A final peak usually occurs between *6pm* and *7pm*, shortly after people return from work.

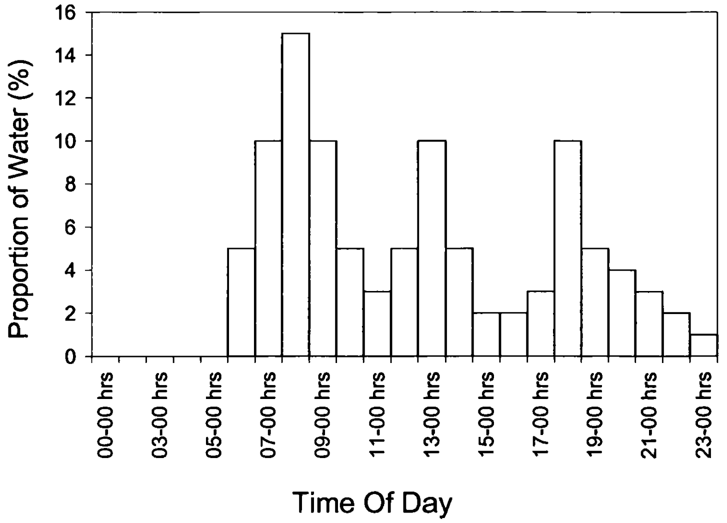


Figure 2.7. Water usage pattern.

The example shown (Figure 2.7) illustrates how the 24-hour day has been discretised into 1-hour time periods. While this is sufficient for depicting the general pattern of water usage, it lacks the resolution required to represent every individual water usage, i.e. every time the tap is turned on. Although, in theory, it is possible to represent the pattern of water usage with a 1-second resolution, it is of little purpose since real-world domestic water usage information at this resolution is scarce. Instead, a more efficient method of dicretising the 24-hour day is to use a resolution that is indicative of the mean inter-use time. Whilst this has been shown [62] to decrease with increasing number of occupants, the average inter-use stagnation time has been found to be about *30 minutes*. However, this includes the overnight stagnation, which is usually about *6 hours*; consequently, the mean inter-use time during the day is considerably shorter, approaching *15 – 20 minutes*.

Since the flow time for the kth time period F_k is:

$$F_k = (P_k/100) \times (V^T/Q) \qquad \text{Eqn. 2.34}$$

where P_k is the percentage of total daily volume of water used in the kth time period. It follows that, for a pattern of water usage discretised into equal time periods, the stagnation time for the kth time period S_k *(sec)*, i.e. the time for which the tap is off, is calculated as:

$$S_k = Y - [(P_k/100) \times (V^T/Q)] \qquad \text{Eqn. 2.35}$$

where Y is the total length of the time period in seconds. The total number of time periods in one day, P is calculated as:

$$P = (24 \times 3600)/Y \qquad \text{Eqn. 2.36}$$

Thus, the complete pattern of water usage for a 24-hour cycle can be described by an alternating series of flow periods and stagnation periods as:

$$YP = \sum_{k=1}^{P} (F_k + S_k) \qquad \text{Eqn. 2.37}$$

This description of a water usage pattern effectively describes the duration of every single flow event and stagnation event that takes place within the pipework during one day. The concentration of lead in the water, contained within the pipework, must be modelled for all events. Mass transfer during stagnation must be modelled during every stagnation event and mass transfer during flow must be modelled during every flow event.

2.2.3 Mass transfer during stagnation

During stagnation there is no flow within the system; consequently, from Eqn. 2.8 it is clear that the only process of mass transfer that can take place is diffusion. Ignoring diffusion along the length of the pipe and assuming concentration in the θ-direction does not vary, the full mass transfer equation Eqn. 2.8 for this case can simplified to:

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{1}{r}\frac{\partial c}{\partial r}\right) \qquad \text{Eqn. 2.38}$$

This equation can be solved analytically or numerically to obtain concentration of lead c as a function of t, r and D.

2.2.3.1 Analytical Solution

2.2.3.1.1 Bessel Function Solution

Eqn. 2.38 is solved subject to the boundary conditions

$$\begin{array}{lll} c = c_0 = E & \text{for } r = r_0, & \text{for } t \geq 0 \\ c = f(r) & \text{for } 0 < r < r_0, & \text{for } t = 0 \end{array} \qquad \text{Eqn. 2.39}$$

where $f(r)$ is the initial concentration distribution across the cross-section of the pipe and E is the equilibrium or maximum concentration of lead in water. For the copper pipe we must set E to the area-weighted average concentration $c_{average}$ (Eqn. 2.40) namely,

$$E = c_{average} = \frac{1}{A}\sum_{j=1,n} a_j \bar{c}_j \qquad \text{Eqn. 2.40}$$

where a is the cross-sectional area for annuli $j = 1,r$ and $\bar{c}_j$ is the average concentration of the edge nodes of annuli $j\text{-}1$ and j.

The solution of Eqn. 2.38 subject to Eqn. 2.39 describes how the concentration varies across the pipe cross-section and is given by [69]

$$c = c_0\left[1 - \frac{2}{r_0}\sum_{n=1}^{\infty}\frac{1}{\alpha_n}\frac{J_0(r\alpha_n)}{J_1(r_0\alpha_n)}\exp\left(-D\alpha_n^2 t\right)\right] + \frac{2}{r_0^2}\sum_{n=1}^{\infty}\exp\left(-D\alpha_n^2 t\right)\frac{J_0(r\alpha_n)}{J_1^2(r_0\alpha_n)}\int_0^{r_0} rf(r)J_0(r\alpha_n)dr$$

Eqn. 2.41

where J_0 and J_1 are Bessel functions and α_n are the positive roots of

$$J_0(r_0\alpha_n) = 0$$

Eqn. 2.42

Thus, the concentration of lead in water after a stagnation period $t = T$ can be calculated assuming the initial conditions are known, i.e. the equilibrium concentration E and the initial concentration distribution across the cross-section of the pipe $f(r)$.

2.2.3.1.2 Issues in the Evaluation of the Solution

It was found that when solving the diffusion problem over small times ($t < 60$ *sec*) the Bessel equation (Eqn. 2.41) produced anomalous results. These consisted of very unrealistically high concentrations during the initial stagnation period; these gradually fell to expected levels after about one minute as shown (Figure 2.8). It should be noted that the expected average concentration within the copper pipe is constant over time during a stagnation period since there is no source term for the copper pipe. Thus the expected average is equal to the initial average obtained from Eqn. 2.40.

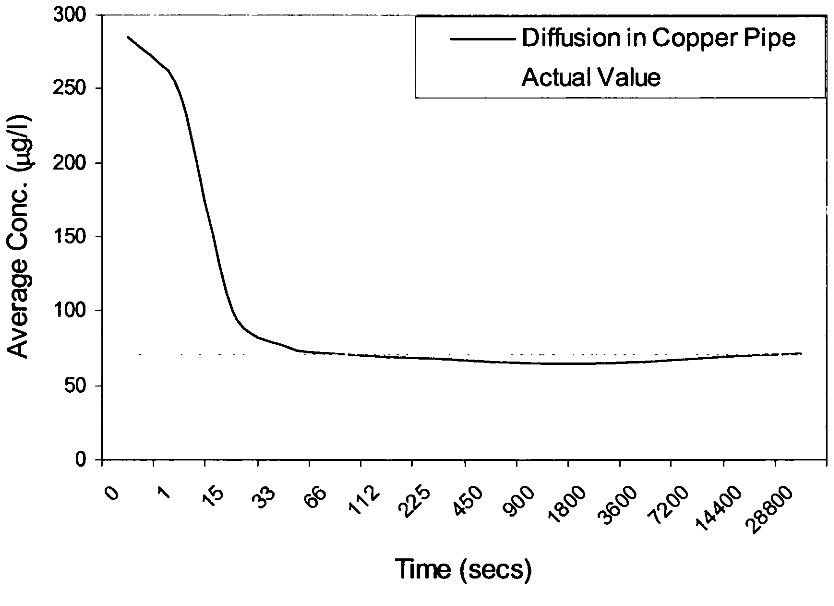


Figure 2.8. Solution of the Bessel equation (copper pipe).

This problem was investigated in some detail [72] and the cause has been traced back to the integral within the Bessel equation (Eqn. 2.41), namely

$$Int = \int_0^{r_0} rf(r)J_0(r\,\alpha_n)dr \qquad \text{Eqn. 2.43}$$

The first 40 α_n values have been obtained from tables [73]. The integral, *Int* has been found for each Bessel root up to *n*. The results have been plotted for $n = 40$ and for increasingly fine radial discretisation, as shown (Figure 2.9).

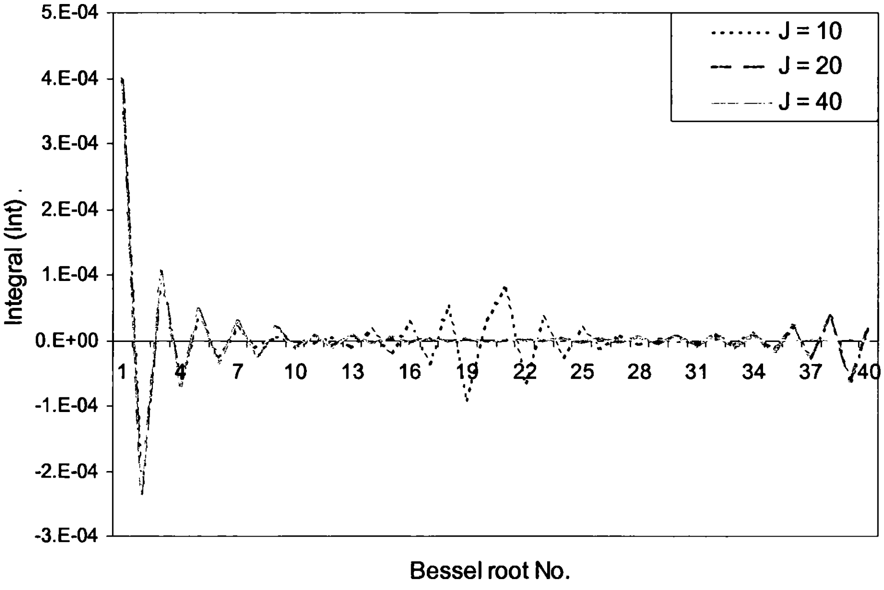


Figure 2.9. Evaluation of the integral *Int* at each Bessel root.

Since the analytical diffusion model must converge to a unique solution, it is clear that, for a particular Bessel root, the integral *Int* must converge to zero as the Bessel root number increases. However, Figure 2.9 reveals that when using 10 radial elements *Int* starts to diverge and then converge again around the 20 Bessel root mark. This instability occurs again around the 40 Bessel root mark for both the 10 and 20 radial element problems. By extrapolation it is possible to predict that *Int* for the 40 radial element problem will undergo a similar instability around the 80 Bessel root mark.

The reasons for these disturbances are not fully understood. Initially it was thought that they were caused by the inaccuracies in the computation of the integral *Int*. However, several increasingly accurate methods, including Trapezoidal, Simpson's and Gauss Quadrature methods have all given similar results. Until further work is done, it is assumed that these disturbances, much akin to some sort of resonance, are caused by the nature of the Bessel functions themselves.

To conclude this particular investigation, a basic rule has been devised in order to prevent anomalous solutions at small times. Consideration of Figure 2.9 reveals that when the integral *Int* has converged, the Bessel root number is the same as the number of radial elements. Therefore, *J* Bessel roots must be used for *J* radial divisions.

Conservation of Mass

As well as the initial anomalous concentration spike, Figure 2.8 also reveals that the Bessel solution is underestimating the average concentration for the copper pipe. The expected average concentration within the copper pipe is constant over time during a stagnation period since there is no source term for the copper pipe. Figure 2.8 shows that the computed average concentration using the Bessel solution immediately drops below the expected value and eventually returns to the expected value after about *25000 sec*. Therefore the Bessel solution is underestimating the mass of lead in the copper pipe as *mass* = *concentration* × *volume*. This implies that the conservation of mass is not being maintained.

This loss in the conservation of mass can be explained by the Bessel equation, or more specifically the boundary conditions used. For the copper pipe, the pipe edge concentration c_0 has been set to the initial area-weighted average concentration $c_{average}$ (Eqn. 2.40) in order that Eqn. 2.41 may be used for the copper pipe. This is a Dirichlet boundary condition, and, in the case of the copper pipe, is discontinuous in nature as the pipe edge concentration effectively jumps from c_0 to $c_{average}$ when applying this boundary condition. Due to the nature of the flow model in most cases the initial $c_{average} < c_0$, therefore the edge concentration c_0 drops. This drop results in the drop in the computed average concentration using the Bessel solution and therefore the loss of the conservation of mass. This problem may be overcome by applying a more suitable Neumann boundary condition for the copper pipe. However, this is not possible when using the analytical solution (Eqn. 2.41), though it may be used in a numerical solution.

Calibration of Diffusion Coefficient

The diffusion coefficient *D* controls the rate of dissolution of lead into the water. If M_t denotes the quantity of lead that has entered or left the cylinder in time *t* and M_∞ the corresponding quantity after infinite time [69], then from (Eqn. 2.41)

$$\frac{M_t}{M\infty} = 1 - \sum_{n=1}^{\infty} \frac{4}{r_0^2 \alpha_n^2} \exp\left(-D\alpha_n^2 t\right) \qquad \text{Eqn. 2.44}$$

and since

$$\frac{c}{E}=\frac{M_t}{M_\infty}$$ Eqn. 2.45

It follows that

$$c=E\left[1-\sum_{n=1}^{\infty}\frac{4}{r_0^2\alpha_n^2}\exp\left(-D\alpha_n^2 t\right)\right]$$ Eqn. 2.46

Thus, suitable values of *D* can be obtained from calibration of Eqn. 2.46 with experimental data. It is clear from Eqn. 2.46 that concentration at any time increases logarithmically with increasing *D*.

2.2.3.2 Numerical Solution

As previously discussed, the Dirichlet boundary condition in the case of the copper pipe is discontinuous and results in a loss in the conservation of mass. As it is not possible to apply a more suitable Neumann boundary condition when using the analytical solution (Eqn. 2.41), a numerical solution can be developed where a Neumann boundary condition is readily applied.

The pipe is treated as a cylinder, which is discretised along the axis (i, $i = 1, N$), and in the radial direction (j, $j = 1, J$) (Chapter 2.2.1.3). The concentration of lead in the pipe c_j^n is defined as

$$c_j^n = c(j\Delta r, n\Delta t)$$ Eqn. 2.47

where Δr is the increment in the radial direction ($\Delta r = r_o/J$) and Δt is the increment in time.

The diffusion equation (Eqn. 2.38) may then be rearranged and written in finite difference form as

$$C_j^n = C_j^{n-1} + \Delta t D\left[\frac{C_{j+1}^{n-1}-2C_j^{n-1}+C_{j-1}^{n-1}}{\Delta r^2}+\frac{C_{j+1}^{n-1}-C_{j-1}^{n-1}}{2r_j\Delta r}\right]$$ Eqn. 2.48

$$\frac{\partial c}{\partial r}=0 \text{ at } r = r_0, \text{ for } t\geq 0$$ Eqn. 2.49

$C = C_0 = E$ at $r = r_0$, for $t \geq 0$ Eqn. 2.50

$\frac{\partial c}{\partial r} = 0$ at $r = 0$, for $t \geq 0$ Eqn. 2.51

This solution (Eqn. 2.48) is 1st order accurate in time and 2nd order accurate in space. The Neumann boundary condition (Eqn. 2.49) is applied at the copper pipe while the Dirichlet boundary condition (Eqn. 2.50) is applied at the lead pipe. We cannot use a Neumann boundary condition for the lead pipe because the rate of dissolution is not constant. It is possible to use the Dirichlet boundary condition (Eqn. 2.50) for the copper pipe as well as the lead pipe, setting E to the average concentration in the copper pipe. However, this produces discontinuity and does not conserve mass as discussed previously. Note that it is also necessary to apply a symmetry condition (Eqn. 2.51) at the middle of the pipe. Solution of these equations reveals that mass is now conserved within the copper pipe where the Neumann boundary condition is applied.

2.2.3.3 Exponential Approximation

As with fluid flow, mass transfer of lead from the lead pipe into the water can be modelled in varying levels of detail. The analytical and numerical solutions to the diffusion problem, described above, very accurately model the real-world response of such a system, as demonstrated by the results from experimental work, described in subsequent chapters (Chapter 2.5). However, these methods are computationally intensive and time consuming due to the complexity of the analytical solution and the $T/\Delta t$ computations required in the numerical solution. Consequently, a simple approximation to the more accurate diffusion solutions will also be considered.

It was deemed that a simple exponential function would approximate well to the real-world diffusion response as depicted by the stagnation curve. This simple approximation assumes that the mass transfer of lead, from the internal surface of a pipe into the water within the pipe, is a function of the initial mass transfer rate M (µg/m^2/s), and the equilibrium concentration of lead in the water, E (µg/l). The source of lead, S (µg/s), is directly proportional to the initial mass transfer rate, i.e. $S \alpha M$. S is also directly proportional to the degree of saturation of lead with respect to E, i.e. $S \alpha (E - c)/E$, thus

$$S = A_S M \frac{(E-c)}{E}$$ Eqn. 2.52

where A_s (m) is the internal surface area of the pipe. Thus, the accumulation of lead within the water at any time t, is given by the equation

$$\frac{dc}{dt}=\frac{A_s M}{V}\frac{(E-c)}{E} \qquad \text{Eqn. 2.53}$$

where V (l) is the volume of the pipe.

By integration of Eqn. 2.53, an expression for the concentration after a stagnation period of length T follows as

$$c=E-(E-c_0)e^{-\frac{A_s MT}{VE}} \qquad \text{Eqn. 2.54}$$

where c_0 is the initial concentration at the start of the stagnation period.

Since this exponential approximation is not dependent on the radial position r, the increase in concentration, due to the mass transfer from the inner wall of the pipe, is only dependant on the initial concentration at that particular radial position. Assuming E is known, M can be calibrated with experimental data [43]. As with D it is clear from Eqn. 2.54 that concentration at any time increases logarithmically with increasing M.

2.2.4 Mass transfer during flow

2.2.4.1 General solution – flow with diffusion

When there is flow within the system, i.e. when the tap is turned on, it is clear from Eqn. 2.8 that both processes of mass transfer will take place because velocity along the pipe u is no longer zero. Thus, lead will enter the water at the inner wall of the lead pipe through the process of diffusion as in stagnation. However, lead will also be transferred along the length of the pipe through the process of advection during flow. Ignoring diffusion along the length of the pipe, which is insignificant, and assuming concentration in the θ-direction does not vary, the full mass transfer equation Eqn. 2.8 for this case can be written as:

$$\frac{\partial c}{\partial t}=-u\frac{\partial c}{\partial x}+D_F\left(\frac{\partial^2 c}{\partial r^2}+\frac{1}{r}\frac{\partial c}{\partial r}\right) \qquad \text{Eqn. 2.55}$$

where D_F is the coefficient of diffusion during flow. The coefficient of diffusion during flow will vary to some extent across the pipe cross-section. The coefficient of diffusion during flow at the location immediately adjacent to the pipe wall is equal to the molecular diffusion coefficient D. However, the coefficient in the central region of the pipe is significantly higher, being dependant on both the molecular diffusion coefficient and the turbulent eddy diffusion coefficient. Turbulent eddy diffusion is the dispersion of a substance due to the mixing action of the fluid in turbulent flow and can be estimated from the flow characteristics and boundary layer thickness using a number of semi-empirical formulae. The effect of turbulent eddy diffusion will be to decrease the concentration gradient in the centre of the flow and thus increase the concentration gradient across the boundary layer. This will have the effect of increasing the quantity of lead that can diffuse into the water during flow to some extent.

However, for simplicity, it will be assumed that D_F is constant across the pipe cross-section and is equal to the molecular diffusion coefficient D since the generation of lead during flow is deemed to be primarily influenced by mass transfer from the pipe wall to the water adjacent to the boundary layer. For completeness, separate diffusion coefficients can be specified in the model for stagnation and flow, e.g. if there is sufficient experimental quantification / verification of D_F.

Depending upon the flow model, the velocity in the pipe is constant for plug flow, or given by (Eqn. 2.17) or (Eqn. 2.22), for laminar and turbulent flow, respectively. Thus, Eqn. 2.55 can be written in finite difference form as:

$$\frac{dC_{i,j}}{dt} = \frac{u_{i,j}}{\Delta x}(C_{i-1,j} - C_{i,j}) + D_F\left[\frac{C_{i,j+1} - 2C_{i,j} + C_{i,j-1}}{\Delta r^2} + \frac{C_{i,j+1} - C_{i,j-1}}{2r_j \Delta r}\right] \qquad \text{Eqn. 2.56}$$

which is then solved using a finite difference representation of the left hand side and time integration by means of a standard approximation method, such as Runge-Kutta or Euler. The Euler approximation, which is first-order accurate and computationally quickest, is written as:

$$C_{i,j}^{n} = C_{i,j}^{n-1} + \Delta t\left\{\frac{u_{i,j}}{\Delta x}(C_{i-1,j}^{n-1} - C_{i,j}^{n-1}) + D_F\left[\frac{C_{i,j+1}^{n-1} - 2C_{i,j}^{n-1} + C_{i,j-1}^{n-1}}{\Delta r^2} + \frac{C_{i,j+1}^{n-1} - C_{i,j-1}^{n-1}}{2r_j \Delta r}\right]\right\} \qquad \text{Eqn. 2.57}$$

where superscripts *n* and *n-1* indicate timestep.

Thus, concentration of lead is computed by applying Eqn. 2.57 on the discretised domain. Concentration in the first axial element along from the water main ($C_{1,j}$) can be computed since the water entering is known to be free from lead, which gives rise to the boundary condition:

$C_{0,j}^{n} = 0 \quad (j = 1, J) \text{ for all } n$ Eqn. 2.58

The concentration in the next axial element (C_{2j}) is then calculated knowing (C_{1j}) and so on, until the concentration at the tap end of the system is computed. Note that this solution is applied to both the lead section of the pipe and the copper section of the pipe. However, in the case of the copper pipe, D_F is set to zero since there is no lead being transferred from the pipe wall to the water here. Consequently, diffusion within the copper pipe is not modelled during flow since the effect on concentration is insignificant compared to that caused by advection.

As previously described, the Dirichlet boundary condition (Eqn. 2.50) and the symmetry condition (Eqn. 2.51) must be applied at the lead pipe.

Since different boundary conditions are applied to the lead pipe and the copper pipe, they may be treated separately. However, it is necessary to set the concentration input at the start of the copper pipe to the concentration at the end of the lead pipe after every timestep.

2.2.4.2 General solution – flow with exponential approximation

Alternatively, the simpler exponential approximation, previously described, may be used in place of the full diffusion equation to describe the mass transfer from the inner wall of the lead pipe:

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} + \frac{A_s M}{V}\frac{(E-c)}{E} \qquad \text{Eqn. 2.59}$$

Once again, this is then solved using a finite difference representation of the left hand side and time integration by means of a standard approximation method, in this case Euler:

$$C_{i,j}^{n} = C_{i,j}^{n-1} + \Delta t\left\{\frac{u_{i,j}}{\Delta x}(C_{i-1,j}^{n-1} - C_{i,j}^{n-1}) + A_{si}\frac{M}{\sum_{j} V_{i,j}}\left[\frac{E - C_{i,j}^{n-1}}{E}\right]\right\} \qquad \text{Eqn. 2.60}$$

where $V_{i,j}$ and A_{si} are the volume of element (i,j) and the internal surface area of element i at the wall of the pipe.

The Runge-Kutta approximation, which is fourth-order accurate and more computationally intensive, is written as:

$$C_{i,j}^{n} = C_{i,j}^{n-1} + \frac{\Delta t}{6}\left(k_{1,i,j} + 2k_{2,i,j} + 2k_{3,i,j} + k_{4,i,j}\right) \qquad \text{Eqn. 2.61}$$

where

$$k_{1,i,j} = \left\{ \frac{u_{i,j}}{\Delta x}(C_{i-1,j}^{n-1} - C_{i,j}^{n-1}) + A_{si}\frac{M}{\sum_{j} V_{i,j}}\left[\frac{E - C_{i,j}^{n-1}}{E}\right] \right\}$$

$$k_{2,i,j} = \left\{ \frac{u_{i,j}}{\Delta x}(C_{i-1,j}^{n-1} - C_{i,j}^{n-1}) + A_{si}\frac{M}{\sum_{j} V_{i,j}}\left[\frac{E - \left(C_{i,j}^{n-1} + \left(k_{1,i,j}/2\right)\right)}{E}\right] \right\}$$

$$k_{3,i,j} = \left\{ \frac{u_{i,j}}{\Delta x}(C_{i-1,j}^{n-1} - C_{i,j}^{n-1}) + A_{si}\frac{M}{\sum_{j} V_{i,j}}\left[\frac{E - \left(C_{i,j}^{n-1} + \left(k_{2,i,j}/2\right)\right)}{E}\right] \right\}$$

$$k_{4,i,j} = \left\{ \frac{u_{i,j}}{\Delta x}(C_{i-1,j}^{n-1} - C_{i,j}^{n-1}) + A_{si}\frac{M}{\sum_{j} V_{i,j}}\left[\frac{E - \left(C_{i,j}^{n-1} + k_{3,i,j}\right)}{E}\right] \right\}$$

As before, concentration of lead is computed by applying either Eqn. 2.60 or Eqn. 2.61 on the discretised domain subject to the boundary condition Eqn. 2.58. Note that this solution is also applied to both the lead section of the pipe and the copper section of the pipe, though in the case of the copper pipe M is set to zero since there is no lead being transferred from the pipe wall to the water here. This is the most appropriate method when used in conjunction with plug-flow, as velocity and concentration do not vary with radial position r in this case. Additionally, it is not necessary to discretise the pipework radially, since the solution Eqn. 2.60 will be independent of r in the case of plug-flow, with variations in concentration along the length of the pipe only.

By utilising this simple method we can effectively treat the pipe as a number of longitudinal elements, each having uniform lead concentration within. The output from the first element within the pipe (i.e. the element at the water mains end of the pipe) is input into the second element and so on until water in the final element in the pipe is output as the concentration at the tap. This is a standard approach widely used in the modelling of water quality of rivers and channels.

2.2.4.3 Analytical solution

In order to validate the results obtained by implementing the solutions, described above, it is necessary to obtain an analytical solution to the problem. In the case of mass transfer during flow, it is possible to develop an analytical solution for the concentration of lead in water under steady-state conditions. Steady-state conditions of such a system are achieved when there is no further variation in concentration with time. In practical terms, this occurs when the water has been flowing through the pipework continuously for a long period of time.

Thus, steady-state conditions are achieved when

$$\frac{dC_{i,j}}{dt} = 0 \text{ for all } i,j \qquad \text{Eqn. 2.62}$$

This is substituted into the finite difference form of Eqn. 2.60 and rearranged to give the analytical solution for $C_{i,j}$ in terms of $C_{i-1,j}$.:

$$C_{i,j} = \frac{\left[\left(\frac{u_{i,j}}{\Delta x}\right)C_{i-1,j} + \frac{A_{si}M}{\sum_j V_{i,j}}\right]}{\left[\frac{u_{i,j}}{\Delta x} + \frac{A_{si}M}{\sum_j V_{i,j}E}\right]} \qquad \text{Eqn. 2.63}$$

By applying the boundary condition Eqn. 2.58 to Eqn. 2.63, the concentration in every element (*i,j*) can be computed for steady-state conditions. This analytical solution will be used to validate the results obtained from the computational model that implements the general flow solutions, described above.

2.2.5 Computing concentration

2.2.5.1 Integrated model

The solutions of mass transfer during stagnation and mass transfer during flow, described previously, are applied to the discretised pipework for a 24-hour pattern of water usage, characterised by a series of alternating stagnation and flow events, as described in Chapter 2.2.2. The concentration of lead in water within the lead pipe is assumed to be zero at the start of the day (midnight). However, at the end of every flow or stagnation event, the computed concentration of lead in every element within the pipework is used as the initial condition for the subsequent flow or stagnation event.

Consequently, every microgram of lead is accounted for throughout the simulated day, and so the concentration of lead at any one time is dependent on all previous water usage in that day. This integrated model can be characterised by the flow diagram illustrated (Figure 2.10).

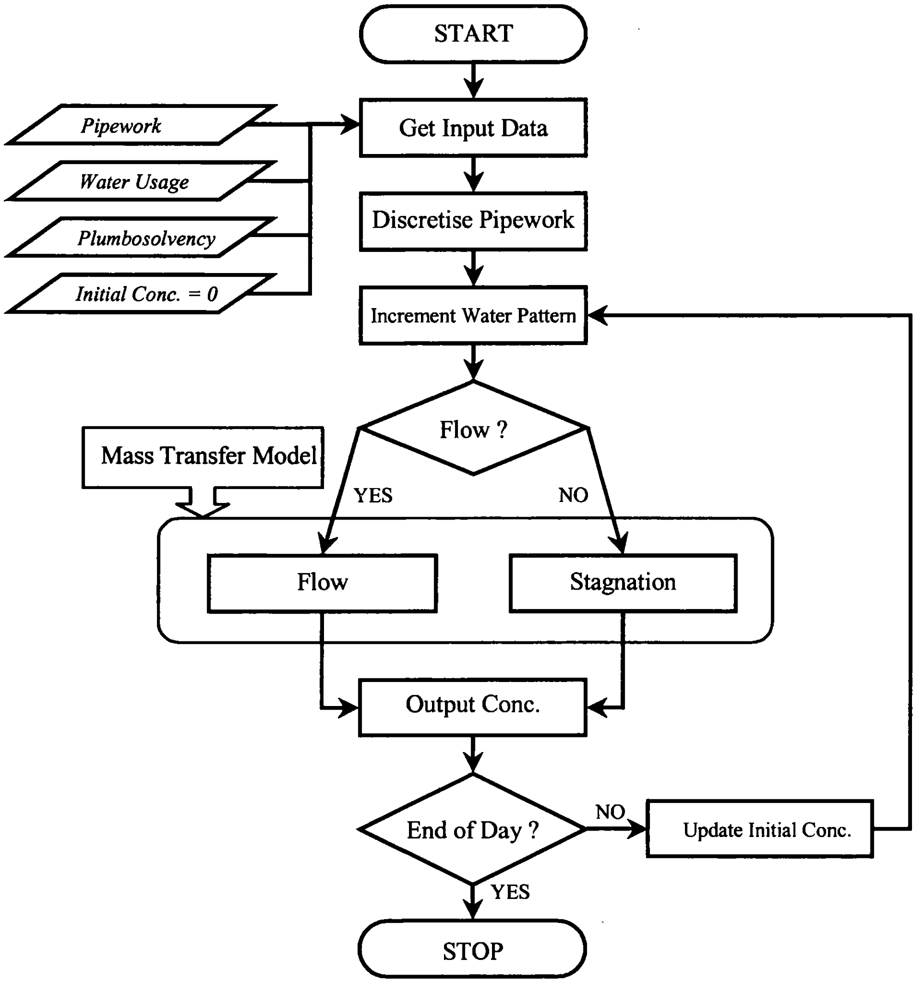


Figure 2.10. Integrated model.

By integrating the solutions of mass transfer with the mathematical representation of the pipework and water usage in this way, it is possible to compute the concentration of lead in water for every element within the pipe, at every second during the day. However, of primary interest is the concentration of lead in the water that is drawn from the tap.

2.2.5.2 Concentration at tap

In the case of plug-flow, concentration at the tap is simply calculated as the concentration in the last element in the copper section of the pipe. However, in the case of laminar and turbulent flow, the pipework is discretised radially, resulting in a concentration variation across the cross-section of the pipe. In order to calculate the actual concentration of lead in the water being output at the tap, it is necessary to calculate an average concentration over the pipe cross-section at the tap for every timestep. This average value is calculated by integrating the product of the concentration and the flow rate over all the radial elements, which comprise the pipe cross-section. This effectively results in a flow-rate-weighted concentration, which is directly linked to the velocity profile and the concentration distribution.

It follows that we may express average concentration $\bar{c}$ as:

$$\bar{c} = \frac{1}{Q}\sum_{j=1,n} u_j a_j c_j \qquad \text{Eqn. 2.64}$$

Where u_j, a_j, c_j are the velocity, cross-sectional area, and concentration of lead for radial element j.

For a radial element of thickness Δr, it is evident that:

$$a_j = 2\pi r_j \Delta r \qquad \text{Eqn. 2.65}$$

For laminar flow, it has been shown that:

$$u_j = \frac{2Q}{\pi r_0^4}\left(r_0^2 - r_j^2\right) \qquad \text{Eqn. 2.66}$$

Thus, from Eqn. 2.64 it follows that, for laminar flow

$$\bar{c} = \frac{1}{Q}\sum_{j=1,n} \frac{2Q}{\pi r_0^4}\left(r_0^2 - r_j^2\right)\left(2\pi r_j \Delta r\right)c_j \qquad \text{Eqn. 2.67}$$

This may be rearranged to give:

$$\bar{c} = \sum_{j=1,n} \frac{4 r_j \Delta r}{r_0^4}\left(r_0^2 - r_j^2\right)c_j \qquad \text{Eqn. 2.68}$$

Similarly, for turbulent flow it can be shown that:

$$\bar{c} = \sum_{j=1,n} \frac{2 r_j \Delta r}{0.817 r_0^2}\left(\frac{r_0 - r_j}{r_0}\right)^{1/7} c_j \qquad \text{Eqn. 2.69}$$

Consequently, it is possible to compute the concentration of lead in the water that is drawn from the tap, for every second during the simulated day, either directly in the case of plug-flow, or by applying Eqn. 2.68 or Eqn. 2.69 for laminar and turbulent flow respectively.

2.2.5.3 Summary statistics

Computing the lead emissions in drinking water throughout a day at a single property produces a vast quantity of data. Whilst output relating to instantaneous lead emissions can be used to investigate factors effecting the temporal variation in lead emissions, it is often more useful to generate a single summary statistic based on the aggregate lead emissions for the single property. The most appropriate statistic to generate is the daily average concentration of lead in drinking water that is drawn from the tap. Daily Average Concentration (*DAC*) is computed as:

$$DAC = \frac{1}{F^T} \sum_{k=1}^{P} \sum_{n=1}^{F_k} \overline{c}^{\,n} \qquad \text{Eqn. 2.70}$$

This allows a single property to be evaluated with respect to lead emissions in accordance with the new "drinking water" directive as the *DAC* computed is also representative of a weekly average value ingested by consumers. Note that the closest real-world equivalent of computing *DAC* is the concentration obtained from composite proportional sampling of a property, described previously.

Summary statistics, such as *DAC*, can be readily employed for investigating how parameters, such as pipework and water usage, effect lead emissions.

2.2.5.4 30-minute stagnation test

By applying a pattern of water use representing a 24-hour period it has been possible to compute lead emissions throughout an entire day as well as an average value. However, using the same principles it is also possible to model the standard "30-minute stagnation" test, widely used in the UK for benchmarking the success of plumbosolvency control treatment (Chapter 1.1.9.1.2). This can be achieved simply by altering the pattern of water usage to represent a stagnation period of 30 minutes, followed by a flow period of sufficient length to allow one litre of water to be drawn from the tap. Additionally, it is necessary to set the initial concentration within the pipework to zero in order to mimic the effect of flushing of the plumbing system, which is carried out to remove as much lead as possible from the water in the pipework. The process of modelling a "30-minute stagnation" test is summarised by Figure 2.11 (*: assumes a flow-rate of $Q = 0.1\ l/s$).

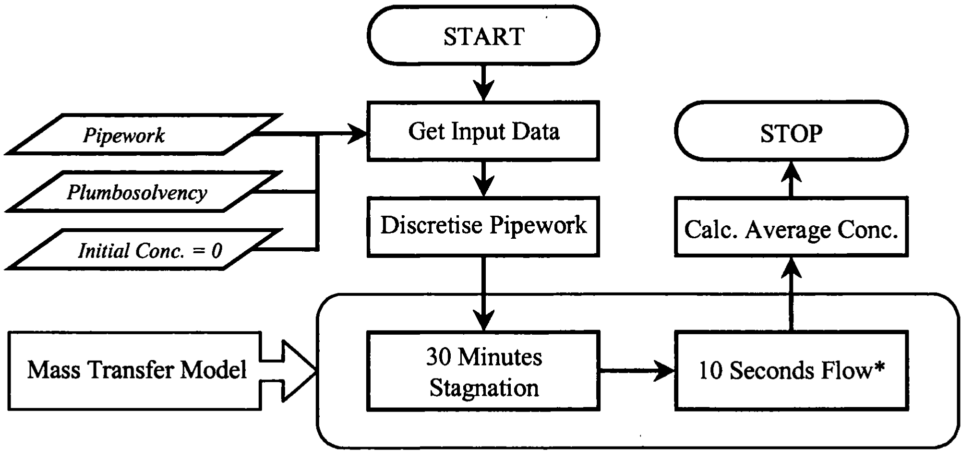


Figure 2.11. Modelling 30-minute stagnation test.

2.2.5.5 Duration of water quality standard breach

It is possible to compare the instantaneous lead emissions at a single property to a specified "water quality standard" (i.e. a standard for lead in drinking water, such as *10*, *25* or *50μg/l*). The total duration that a specified water quality standard is breached in the 24-hour simulation period can be computed. This is achieved simply by comparing the concentration at the tap to the specified standard for every second during the simulated day, and counting how many times $C_{tap} > C_{standard}$. Although this will result in an aggregate of data, it is representative of a total rather than an average value such as *DAC*. Consequently, the duration of breach does not 'smooth out' the data but takes into account the instantaneous peak lead emissions that occur at the property throughout the simulated day.

2.2.6 FORTRAN implementation

The primary objective of this research was to develop a computational model, to be used by water engineers, to investigate the issues that relate to plumbosolvency control. In order to incorporate the flexibility to investigate a wide range of scenarios, the integrated model for computing lead emissions at a single house, has been implemented in a user-operated computer program, developed using FORTRAN.

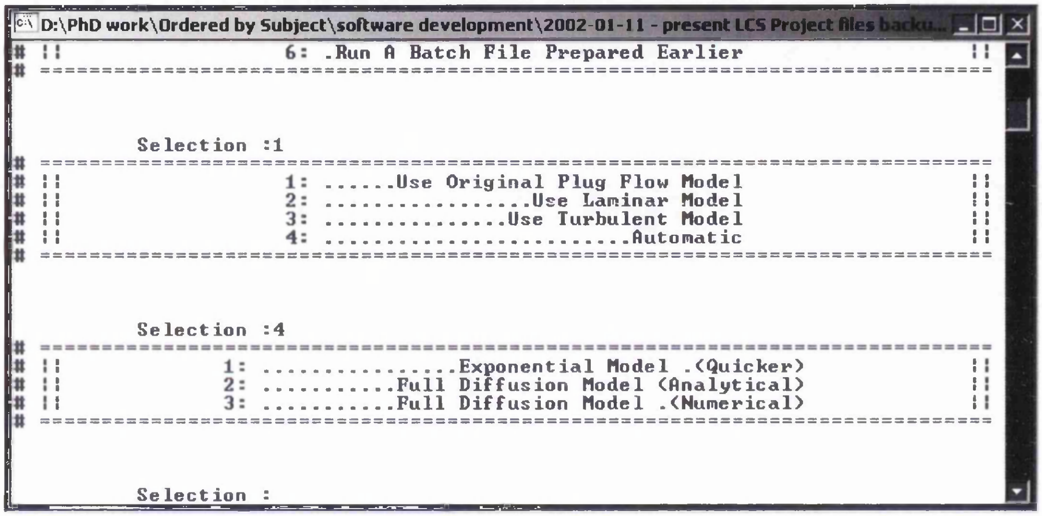
2.2.6.1 Model input

Parameters required by the model include the geometry of the pipework, the water usage and the plumbosolvency of the water:

- Length of Lead Pipework
- Length of Copper Pipework
- Diameter of Pipework

- Flow Rate (when the tap is on)
- Total Volume of Water Used (in one day)
- Pattern of Water Usage
- Plumbosolvency parameters (*M* and *E* or *D* and *E*)
- Water Quality Standard (i.e. a standard for lead in drinking water, such as *10*, *25* or *50µg/l*)

These parameters are input into the model, either through a data file or directly by the user through the software's text menu system. Additionally, the user is asked to specify the flow model and the mass transfer model that will be used (Figure 2.12).



```
# !!                    6: .Run A Batch File Prepared Earlier                 !!
# ============================================================================


        Selection :1
# ============================================================================
# !!                    1: ......Use Original Plug Flow Model                 !!
# !!                    2: .................Use Laminar Model                 !!
# !!                    3: ...............Use Turbulent Model                 !!
# !!                    4: ..........................Automatic                 !!
# ============================================================================


        Selection :4
# ============================================================================
# !!               1: ................Exponential Model .(Quicker)            !!
# !!               2: ...........Full Diffusion Model (Analytical)            !!
# !!               3: ...........Full Diffusion Model .(Numerical)            !!
# ============================================================================


        Selection :
```

Figure 2.12. User options within the software.

This option allows the user to specify how accurately the physical processes of flow and mass transfer should be modelled. Clearly, the plug-flow model coupled with the exponential model of mass transfer will be considerably faster to execute than any other combination of models, since these are the most straightforward mathematically and require no radial discretisation of pipework. Thus, this will be the preferred option when time is more important than accuracy. Conversely, the most physically accurate, yet most computationally intensive combination of models is the turbulent flow model coupled with the numerical diffusion model.

Note also that the user can specify the "automatic" option within the flow model menu (Figure 2.12), which determines the most appropriate flow model (laminar *or* turbulent) to use, based on the Reynolds number. The combination of models that can be specified is illustrated (Figure 2.13).

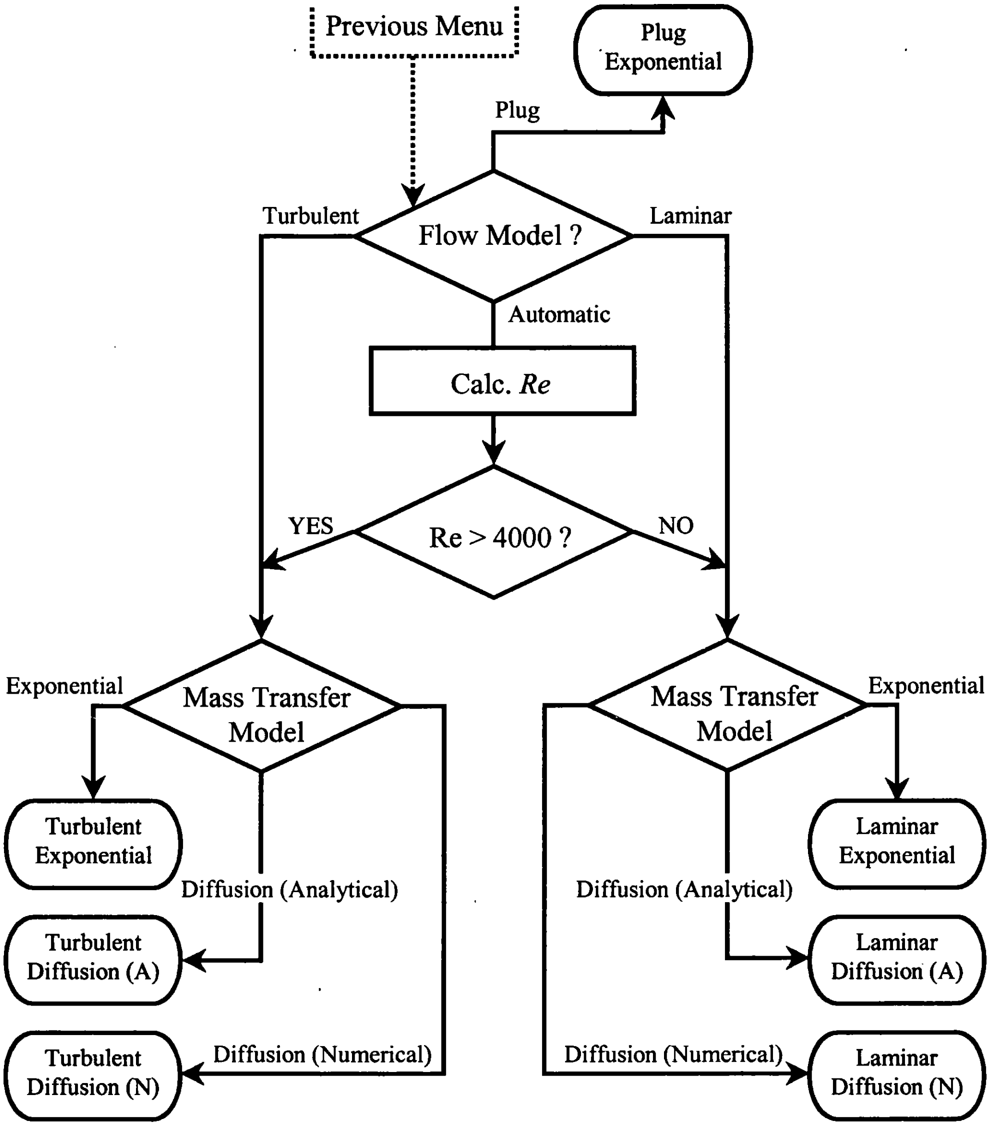


Figure 2.13. Model selection process.

2.2.6.2 General algorithm

The FORTRAN code that has been developed to implement the integrated model for lead emissions at a single house is able to compute concentration of lead throughout the day as well as summary statistics. The code is characterised by the general algorithm:

```
USER INPUT
  • Input Parameters for the single house
  • Input Flow and Mass transfer model
  • Discretise Pipework

SIMULATE ONE DAY
  • Set initial concentrations to zero
  • For every time period in the day ($k = 1,P$)
      Compute concentrations in all elements in pipework after stagnation period $S_k$:
        o For every element in Lead section ($i,j$)
            ▪ Compute: concentration (using mass transfer during stagnation)
        o Next element
        o For every element in Copper section ($i,j$)
            ▪ Compute: concentration (using mass transfer during stagnation)
        o Next element
      Compute concentrations in all elements in pipework during flow period $F_k$:
        o For every second in flow period ($n = 1,F_k$)
            ▪ For every element in the Lead section ($i,j$)
                • Compute: concentration (using mass transfer during flow)
            ▪ Next element
            ▪ Set input of Copper section to Output of Lead section
            ▪ For every element in the Copper section ($i,j$)
                • Compute: concentration (using mass transfer during flow)
            ▪ Next element
            ▪ Compute: average concentration at tap, $\overline{C}$
            ▪ Check to see if $\overline{C}$ exceeds water quality standard
        o Next second
        o Compute (& Output): Max, Min & Average concentration at tap for this time period
        o Compute (& Output): Time water quality standard is exceeded for this time period
  • Next time period
  • Compute (& Output): DAC (Daily Average Concentration at the tap)
  • Compute (& Output): Total time water quality standard is exceeded in 24-hour day

SIMULATE 30-MINUTE STAGNATION
  • Set initial concentration to zero
  • Compute concentrations in all elements in pipework after 30 minute stagnation period
  • For every second in flow period (10 seconds assuming $Q = 0.1$ litres/sec)
      o Compute: average concentration at tap, $\overline{C}$ in the same way as above
  • Next second
  • Compute (& Output): Average concentration at tap for this time period
```

Figure 2.14. General algorithm.

2.2.6.3 Model output

The computational model is able to compute and output a range of parameters relating to the daily lead emissions at the property specified by the input parameters. Highly detailed data, such as the concentration in each element of the pipework for every second throughout the 24-hour simulation period, can be output in the form of a data file. More general parameters that are output include:

- *DAC* (Daily Average Concentration at the tap)
- *30MS* ("30-Minute Stagnation" test result)

- The total time that a specified “water quality standard” is exceeded in the 24-hour simulation period

Additionally, the following parameters are output for each Flow Period in the 24-hour simulation period:

- Length of Flow Period
- Maximum Concentration of Lead at the Tap
- Minimum Concentration of Lead at the Tap
- Average Concentration of Lead at the Tap
- The time that a specified “water quality standard” is exceeded

2.3 Results for a single house

2.3.1 Stagnation

The factors that influence lead emissions at a single property must be investigated in order to understand the general issues that relate to plumbosolvency control. However, it is first necessary to understand how the mass transfer models function under specified conditions, in terms of how the concentration varies temporally and spatially within the pipework. Mass transfer during stagnation can be modelled in varying levels of detail, as previously described. Thus, it is also necessary to investigate how the solutions to each model differ and what implications this may have on predicting lead emissions at a single property.

The solutions obtained from the mass transfer models, illustrated within this subchapter, are obtained by using the following parameters:

Pipework (internal diameter): *12mm*
No. of radial elements, J: *40*
Equilibrium concentration, E: *150μg/l*
Initial mass transfer rate, M: $0.1\mu g/m^2/s$
Diffusion coefficient, D: $4.96E\text{-}10m^2/s$
Timestep, Δt: *1 sec*

Note: The E, M and D values are obtained by calibrating the models to the data point of *50μg/l* at *30 minutes* and assuming a solubility of *150μg/l*, which is representative of a moderately plumbosolvent water.

2.3.1.1 Diffusion models

Solutions from both the analytical and numerical diffusion models exhibit concentration variations across the cross-section of the pipe. This can be illustrated by the solution obtained through the modelling of a stagnation period of 6 hours in a lead pipe with an initial concentration of zero (Figure 2.15). The plot clearly shows the radial variation in concentration and how the lead diffuses from the pipe wall into the middle of the pipe until a maximum concentration E is almost reached across the entire cross-section of the pipe. Note how quickly the concentration of lead increases in the region close to the pipe wall.

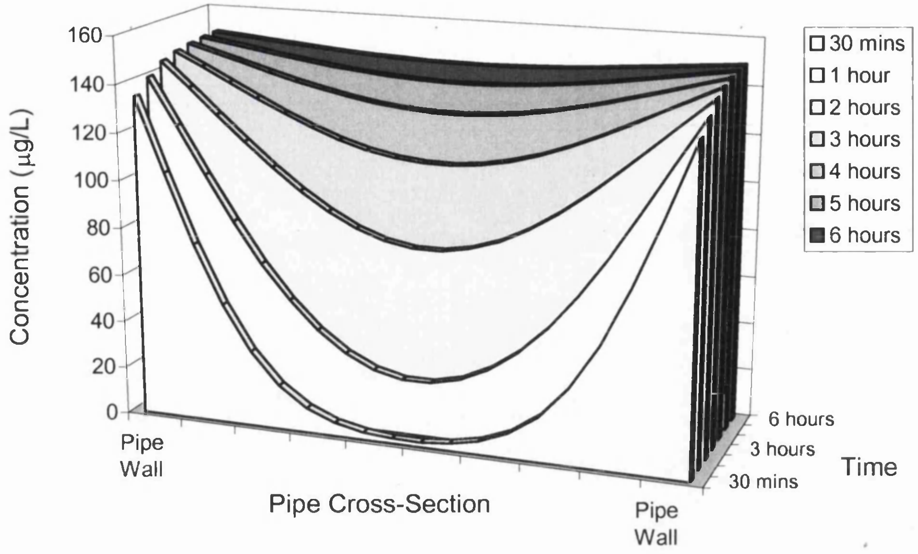


Figure 2.15. Diffusion response during stagnation (lead).

Concentration variations across the cross-section of the pipe can also be illustrated by the solution obtained through the modelling of a stagnation period in a copper pipe with a set non-uniform initial concentration (Figure 2.16). In this case the plot clearly shows how the lead diffuses from the water with the highest concentration (closer to the pipe wall) into the water with the lowest concentration (middle of the pipe), until a uniform concentration is almost reached across the entire cross-section of the pipe after *120 minutes*. This uniform concentration is equivalent to the average concentration across the cross-section of the pipe at the start of the stagnation period. Also note that this solution was obtained from the numerical diffusion model, which applies the Neumann boundary condition (Eqn. 2.49) in the case of the copper pipe.

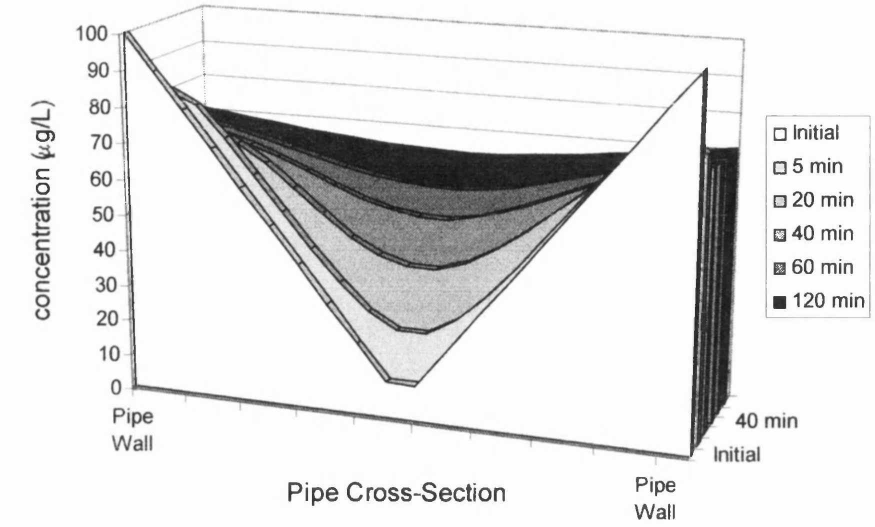


Figure 2.16. Diffusion response during stagnation (copper).

The response of the diffusion models in the case of the lead pipe can also be illustrated by a stagnation curve. However, in this case it is necessary to compute the average concentration of lead across the cross-section of the pipe $C_{average}$ using Eqn. 2.40. The resulting stagnation curve (Figure 2.17) illustrates how the responses of the analytical and numerical diffusion model are practically identical. Although the numerical diffusion model is computationally slower than the analytical diffusion model, it is able to represent the diffusion of lead within the copper pipe accurately and maintains the conservation of mass.

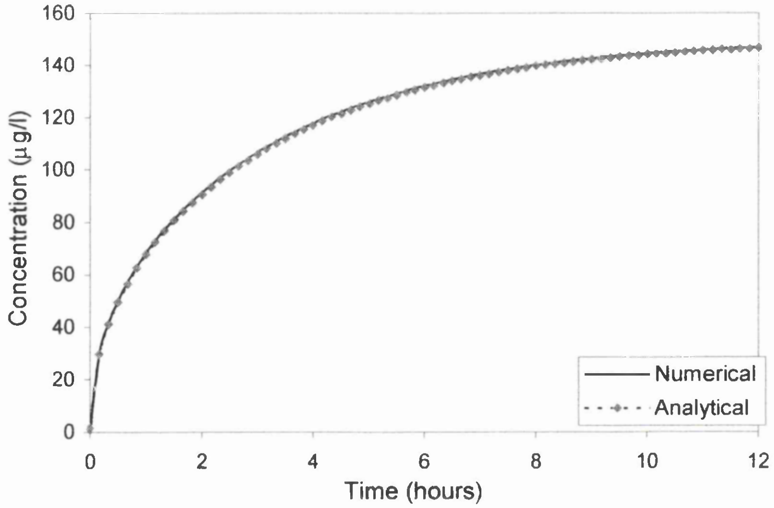


Figure 2.17. Stagnation curves from diffusion models.

2.3.1.2 Non-zero initial concentration

For non-zero initial concentration within the lead pipe, the response of $C_{average}$ from both numerical and analytical diffusion models approximately follows the stagnation curve from the point representing the initial $C_{average}$ in Figure 2.17. However, the response of $C_{average}$ will not follow the remaining stagnation curve exactly unless the initial concentration distribution across the cross-section of the pipe c_j is exactly the same as that arising from a stagnation from an initial concentration of zero. Fick's law states that the flow of mass is proportional to the concentration gradient of the diffusant across that plane, thus the rate of mass generation through the process of diffusion must be dependant on the initial concentration distribution.

An example of the response of $C_{average}$ from the diffusion models for non-zero initial concentration is illustrated (Figure 2.18).

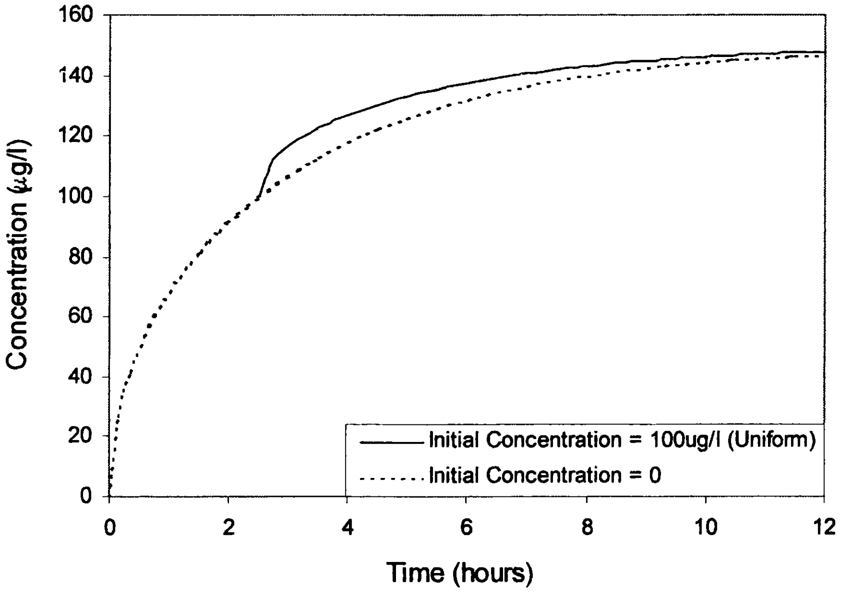


Figure 2.18. Non-zero initial concentration.

In this case the initial concentration is set to *100µg/l*, uniformly applied across the entire cross-section of the pipe, which equates to the $C_{average}$ occurring after a stagnation period of *2.5 hours* from an initial concentration of zero. During stagnation from zero initial concentration, lead diffuses from the pipe wall into the middle of the pipe, resulting in the concentration variation illustrated (Figure 2.15). After *2.5 hours* stagnation, the concentration near the wall of the pipe is considerably higher than $C_{average}$ and thus the concentration gradient here is smaller than that obtained from a uniform concentration of $C_{average}$. Since the wall of the lead pipe is the source of the diffusant, it follows that the generation of lead is slowed in accordance with Fick's law, producing the standard stagnation curve (dotted line, Figure 2.18). The additional lead generated as a consequence of the larger concentration gradient associated with a uniform concentration across the cross-section of the pipe is depicted as the difference between the two curves (Figure 2.18).

2.3.1.3 Exponential Approximation

Solutions from the exponential approximation for mass transfer during stagnation do not exhibit concentration variations across the cross-section of the pipe when the initial concentration is zero. However, when this model is used in conjunction with laminar and turbulent flow and radial discretisation must be applied, the exponential function is effectively applied at each radial position independently. Consequently, for a non-uniform initial concentration across the cross-section of the pipe, the solution will exhibit radial variation, though this variation will decrease with stagnation time (Figure 2.19).

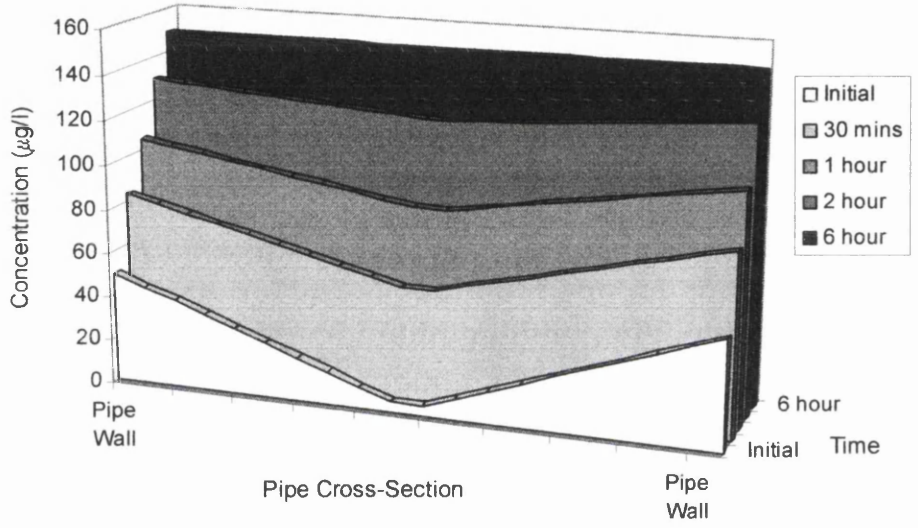


Figure 2.19. Exponential response for non-zero initial concentration.

As with the diffusion models previously discussed, the response of the exponential approximation can also be illustrated by a stagnation curve (Figure 2.20). This illustrates how $C_{average}$ increases with stagnation time and is compared with a corresponding result obtained from the analytical diffusion model. In this case both models are calibrated to the data point of *50μg/l* at *30 minutes* and assuming a solubility of *150μg/l*, these being obtained from experimental data. Consequently, both curves pass through the *30-minute* data point and asymptote to *150μg/l*.

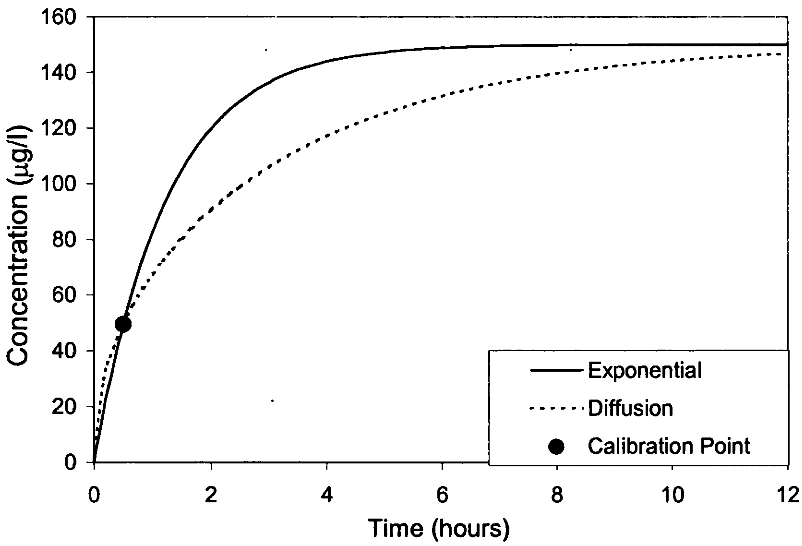


Figure 2.20. Stagnation curve from Exponential approximation.

Although the general shape of the curves are similar, it is clear that the rate of lead dissolution in the case of the exponential model is higher than that for the diffusion model for stagnation times greater than 30 minutes but slightly lower for stagnation times less than 30 minutes. This discrepancy is most apparent between 3 and 4 hours stagnation where the exponential approximation overestimates the concentration by approximately 20%. However, although the discrepancy in the first 30 minutes is not as obvious, the exponential approximation has been found to under-estimate the concentration by approximately 50% at the 10 minutes position.

Since the mean inter-use stagnation time for a residential property has been found to be approximately *15 – 20 minutes* during the daytime, the exponential approximation is expected to underestimate daily lead emissions.

2.3.2 Flow

As well as investigating mass transfer during stagnation, it is also necessary to understand how the models for fluid flow, in conjunction with the models for mass transfer during flow, function under specified conditions, in terms of how the concentration varies temporally and spatially within the pipework. Fluid flow, and consequently mass transfer during flow, can be modelled in varying levels of detail, as previously described. Thus, it is also necessary to investigate how the solutions to each model differ and what implications this may have on predicting lead emissions at a single property.

The solutions obtained from the mass transfer models, illustrated within this subchapter, are obtained by using the following parameters:

Pipework (internal diameter):	*12mm*
Pipework (length of lead):	*10m*
Pipework (length of copper):	*10m*
No. of radial elements, *J*:	*10*
Equilibrium concentration, *E*:	*150μg/l*
Initial mass transfer rate, *M*:	*0.1μg/m*^{2}*/s*
Diffusion coefficient, *D*:	*4.96E-10m*^{2}*/s*
Volumetric flow rate, *Q*:	*0.1l/sec*
Timestep, *Δt*:	*1 sec*

2.3.2.1 Flow immediately after stagnation

When the tap is open, the concentration of lead in the water drawn is either a reflection of the steady state flushed condition or a condition influenced by the previous stagnation, as determined by pipe geometry and the extent of the flow event. Solutions obtained from a flow event immediately after a period of stagnation will be presented and explained within this subchapter.

2.3.2.1.1 Concentration at end of lead pipe

Ultimately, the only point in the pipework that must be monitored to determine lead emissions is the end of the copper pipework (location of the tap). However, investigating other locations in the pipework can provide valuable insight into how the flow and mass transfer models interact throughout the pipework.

Solutions obtained when using the laminar and turbulent flow models exhibit concentration variations across the pipe cross-section. This can be illustrated by the solution obtained through the modelling of a flow period of length *30 seconds* directly after a stagnation period of *6 hours* (Figure 2.21). This particular situation is only likely to occur during 'first draw', i.e. when water is first drawn from the tap in the morning after overnight standing, or alternatively when water is first drawn from the tap when the occupant returns from work, assuming the property is vacant during the day. However, since the concentration of lead within the lead pipe has effectively reached equilibrium *E*, the resulting solution is able to illustrate the full extent of the concentration variations within the pipe that occur during flow. The solution illustrated is obtained when the laminar flow model is used and the plot corresponds to concentrations at the end of the lead pipework.

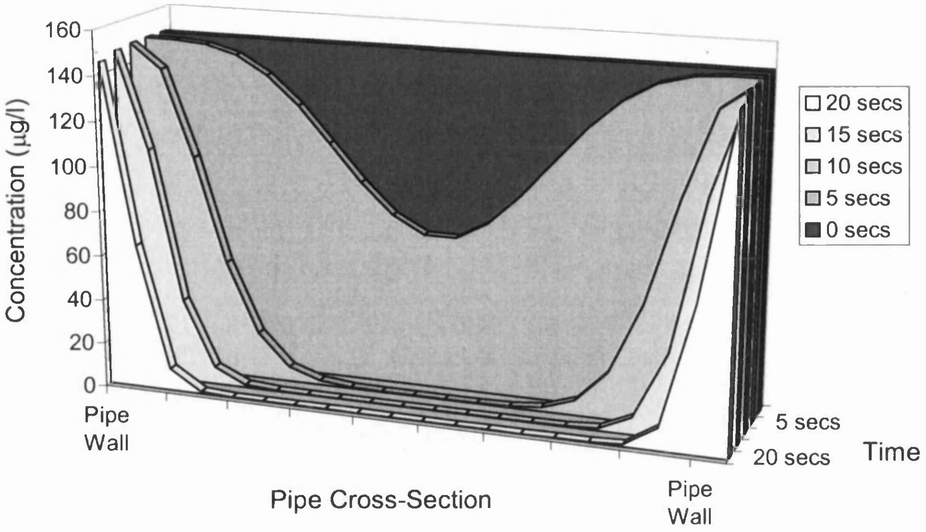


Figure 2.21. Concentration at end of lead pipe during laminar flow.

Observing Figure 2.21 it is clear that the concentration at the start of the flow period is practically uniform across the pipe cross-section since equilibrium conditions have effectively been reached. After *5 seconds* the concentration in the middle of the pipe begins to drop rapidly. This is effectively caused by the 'flushing effect' where fresh water from the water main, which has zero lead content, begins to reach the end of the lead pipework, diluting and effectively flushing out the lead saturated water. Note that this flushing effect first occurs in the middle of the flow because the flow is fastest here. In the laminar model the flow close to the pipe wall is extremely slow, as described by its velocity profile. Hence, even after *20 seconds* the 'flushing effect' has yet to occur here and so the concentration near the pipe wall is still very high. Over a longer period of flow, the concentration near the pipe wall eventually decreases, though much more slowly than in the middle of the pipe.

The corresponding solution obtained when the turbulent flow model is used (Figure 2.22) appears to be quite different to those for the laminar model. The concentration distribution is still uniform after *5 seconds* because the maximum fluid velocity in turbulent flow is approximately 90% slower than that for the laminar model. Consequently, it takes longer for the 'flushing effect' to be noticed at the end of the lead pipe. Note that the concentration close to the pipe wall decreases with time much more quickly in the turbulent model: after just *20 seconds*, all of the lead saturated water in the lead pipe has effectively been flushed out. This is due to the velocity profile of turbulent flow, where the velocity across most of the pipe cross-section is relatively uniform, only diminishing very close to the pipe wall.

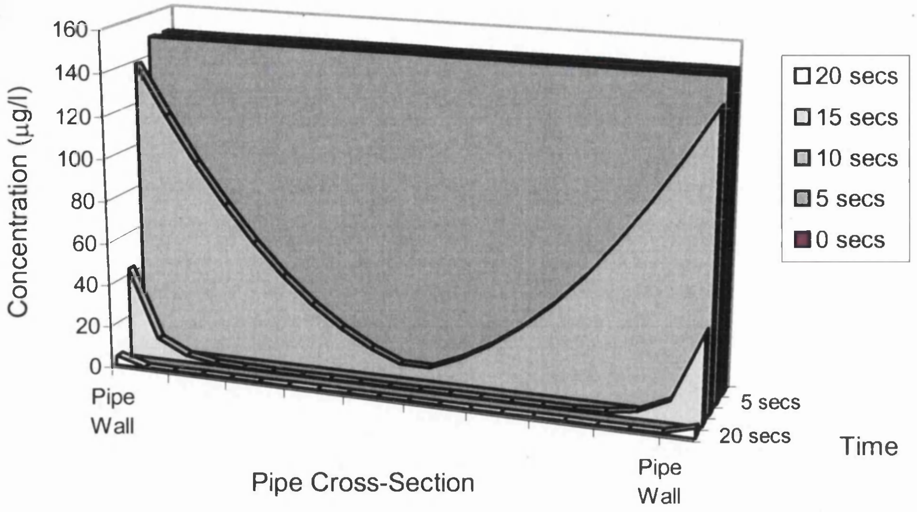


Figure 2.22. Concentration at end of lead pipe during turbulent flow.

2.3.2.1.2 Concentration at tap

Solutions may also be obtained for concentrations at the end of the copper pipe (location of the tap) for the same situation. The solution illustrated (Figure 2.23) is obtained when the laminar flow model is used. The concentration within the copper pipework at the start of the flow period is approximately zero assuming the pipework was adequately flushed prior to stagnation since no lead is generated within the copper during stagnation. Consequently, it takes approximately *5 seconds* for the lead saturated water in the middle of the pipes cross-section to travel through the *10m* copper pipework, from the end of the lead pipework to the tap. After *15 seconds* the 'flushing effect' is apparent in the middle of the pipe as fresh water from the water main dilutes the leaded water. As the 'flushing effect' in the middle of the pipe transpires the opposite occurs near the pipe wall, i.e. the concentration increases. This is due to the flow near the pipe wall being extremely slow compared to the flow in the middle of the pipe. Hence, it takes far longer for the leaded water to reach the tap and consequently far longer for the "flushing effect' to occur here.

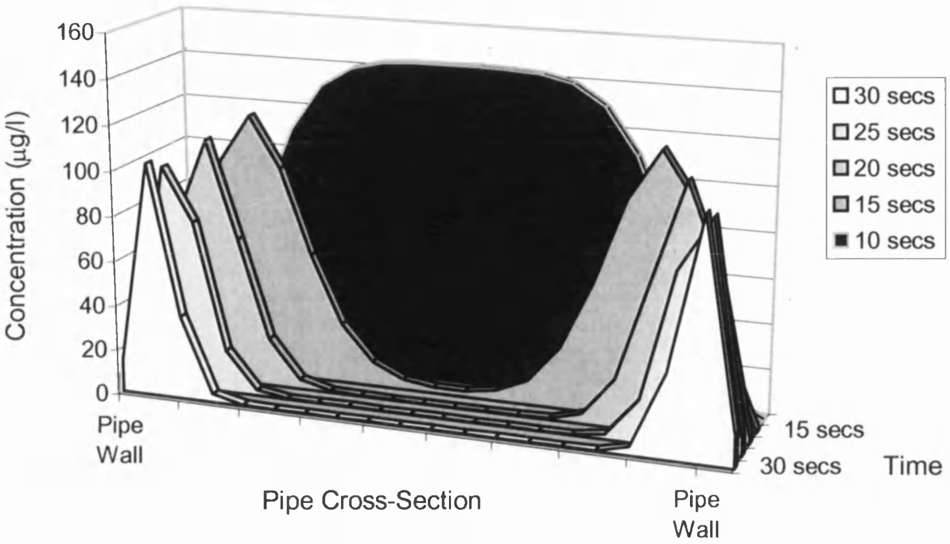


Figure 2.23. Concentration at tap during laminar flow.

The corresponding solution obtained when the turbulent flow model is used has similar characteristics to the laminar solution, though the 'flushing effect' takes longer to commence since the maximum fluid velocity is slower for turbulent flow. However, as before, the 'flushing effect' transpires faster near to the pipe wall than for laminar flow due to the velocity profile.

Solutions for the volume averaged concentration at the tap (Eqn. 2.64) for the different flow models in conjunction with the different mass transfer models are shown (Figure 2.24). The solutions were obtained for the first *45 seconds* of flow after a stagnation period of *4 hours*.

As expected, in turbulent flow, the boundary layer effects are limited to close to the pipe wall and hence the concentration profile is similar to that of plug flow, which does not have a boundary layer. The concentration profile for laminar flow peaks sooner since the maximum velocity is higher; however, the subsequent 'tail end' of the curve reflects the significant boundary layer thickness. It should be noted that the flow within a pipe for typical residential use is likely to be turbulent with laminar flow only likely to occur during periods of very low flow. Note that the peak concentration is lower when the diffusion model is used because the exponential model over-estimates the concentration for stagnation times greater than *30 minutes*, as previously discussed.

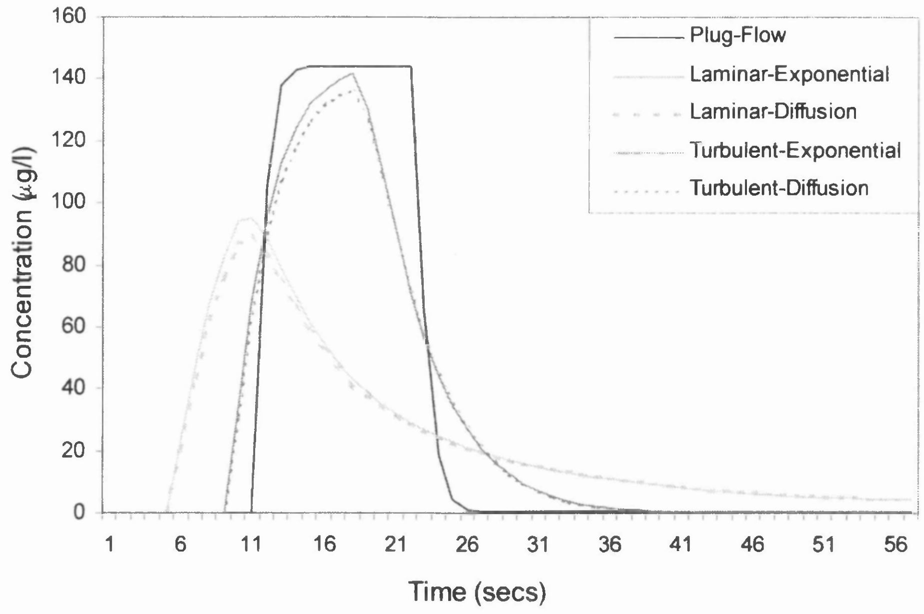


Figure 2.24. Volume averaged concentration at tap during flow.

The area under each curve represents the total amount of lead discharged at the tap. Calculation show that the area under each curve for the exponential model is equal, and the area under each curve for the diffusion model is equal; this in itself confirms that the conservation of mass is consistent for the various models.

2.3.2.2 Steady state concentration

Steady-state conditions are achieved when there is no further variation in concentration with time. In practical terms, this occurs when the water has been flowing through the pipework continuously for a long period of time. The quantity of lead in the water that is output at the tap during steady-state conditions is solely generated through the process of mass transfer during flow. From Figure 2.24, it is clear that steady-state conditions are effectively reached after *30 seconds* and *40 seconds* when using plug flow and the turbulent flow respectively. The resulting steady-state concentration in these cases is approximately *0.5μg/l*. However, since it takes up to *10 minutes* for steady-state conditions to be reached in laminar flow, due to the significant boundary layer thickness, the steady-state concentration may never be reached under typical residential water use.

It is possible to model extended periods of flow and thus obtain a solution for the steady-state concentration for each flow type, including laminar. These numerical solutions can be compared to the analytical solution for steady-state conditions (Eqn. 2.63), previously described, thus enabling validation of the computational model.

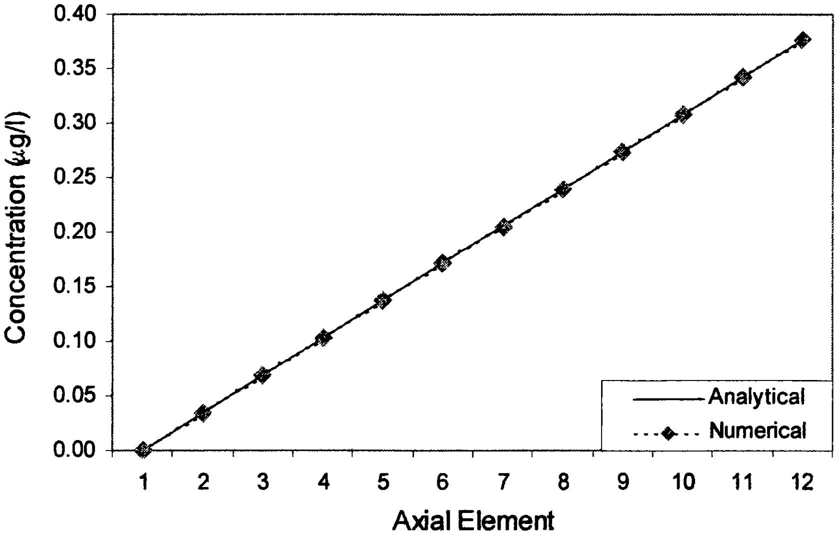


Figure 2.25. Steady-state concentration for plug flow.

Numerical and analytical solutions for the steady-state concentration for plug flow have been obtained for each axial element in a lead pipe of *10m* (Figure 2.25). This clearly illustrates that the computational error, i.e. difference between numerical and analytical solutions, within each axial element of the lead pipe is zero. Consistent results have been obtained for laminar and turbulent flow using both Euler and Runge-Kutta approximations. Note that under steady-state conditions, the concentration increases linearly in the axial direction from zero, where the lead pipe connects to the water main, to a maximum at the end of the lead pipe.

Steady-state concentration variations across the pipe cross-section at the tap reveal the influence of the turbulent flow velocity profile (Figure 2.26). The steady-state concentration increases from a minimum at the centre of the pipe to a maximum at the pipe wall. This is because the slower flow, towards the edge of the pipe, has greater contact time with the lead pipe and is thus able to dissolve a greater quantity of lead. Note also that the steady-state concentration at the edge of the pipe will take longer to achieve than that at the centre of the pipe.

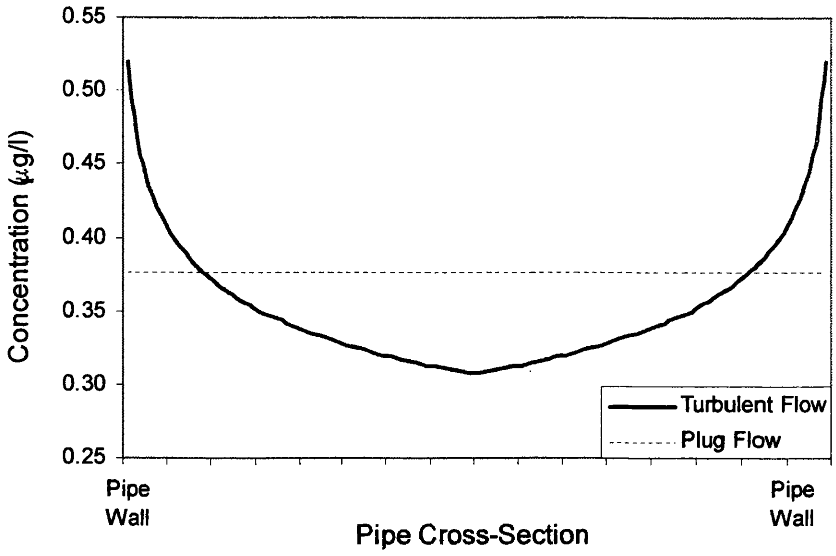


Figure 2.26. Concentration variation across pipe during steady-state.

2.3.3 Daily variation

Solutions, obtained from the various flow and mass transfer models developed, have been investigated for a number of individual situations, including flow periods and stagnation periods, as previously described. The knowledge acquired will facilitate the understanding of the solutions obtained through the modelling of a 24-hour period at a single property.

In order to model lead emissions over the course of an entire day, it is necessary to specify how the water is used throughout the day. Consequently, for the purposes of investigating daily variation of concentration, a pattern of water usage of the form depicted in Figure 2.7, having an inter-use time of $Y = 15$ *minutes* has been applied. Note that this pattern is representative of a property having one or more occupants at home during the working day.

Figure 2.27 shows the solution obtained for concentration at the tap (during flow) over a *24-hour* period, obtained using the plug flow - exponential model, with the assumed water usage pattern. In this example the following parameters have been used:

Pipework (internal diameter):	*12mm*
Pipework (length of lead):	*10m*
Pipework (length of copper):	*10m*
Equilibrium concentration, E:	*150μg/l*
Initial mass transfer rate, M:	$0.1\mu g/m^2/s$

Volumetric flow rate, *Q*: *0.1l/sec*
Daily water consumption: *450l*
Water usage pattern: *15-minute frequency*

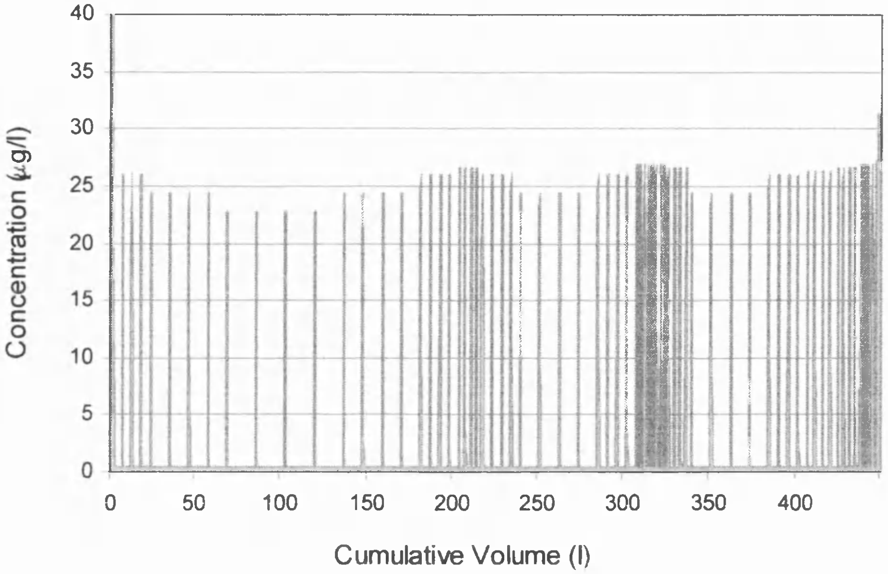


Figure 2.27. Daily concentration variation (10m lead) using plug flow.

The solution clearly demonstrates that, over a *24-hour* period, the concentration of lead in the water drawn from the tap is characterised by an alternating series of high peaks and very low baseline concentrations. The peaks represent the high concentrations obtained near the start of the flow periods, where the water that had previously stagnated in the lead pipework is drawn through the tap. In the case of *10m* lead pipework, each peak lasts approximately *10 seconds*. The low baseline portions represent the steady-state concentration that is achieved after approximately *30 seconds* of continuous flow.

Note that this solution is for the concentration at the tap during flow only. If the solution represented concentration at the tap during the entire day, i.e. including periods of stagnation, then the plot would incorporate very long periods of zero concentration between each flow period. Consequently, the area under the graph represents the total quantity of lead *(µg/l)* drawn from the tap during the simulated day.

The corresponding solution obtained using laminar flow as opposed to plug flow is illustrated (Figure 2.28). Once again, the concentration of lead in the water drawn from the tap is characterised by an alternating series of peaks and troughs. However, there are some important distinctions between the two solutions, namely the peaks and troughs are not as extreme, i.e. there is less variation in concentration throughout the simulated day. In fact, on close inspection, it is apparent that the duration of the actual peak concentrations is smaller and that the steady-state concentration is never fully achieved. This is a direct result of the significant boundary layer thickness found in laminar flow as previously discussed.

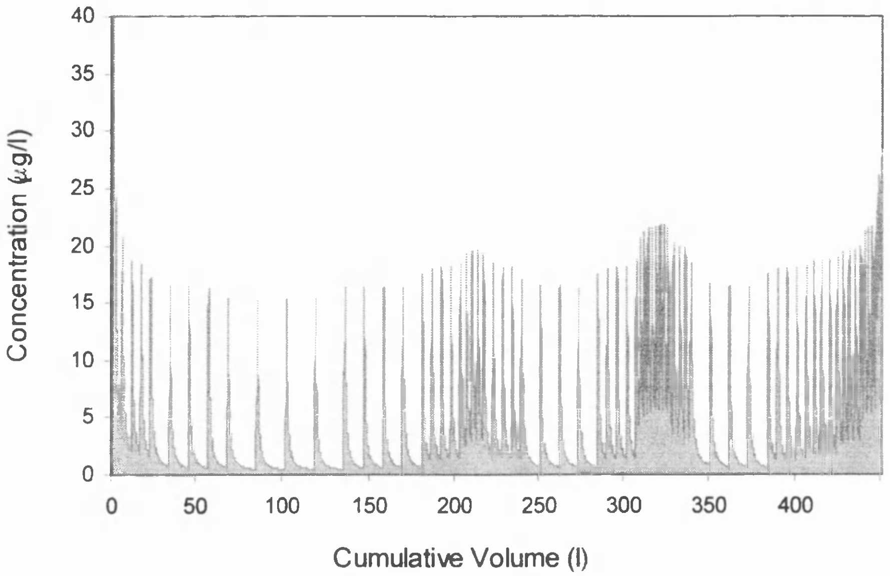


Figure 2.28. Daily concentration variation (10m lead) using laminar flow.

The solution (Figure 2.28) also illustrates how the concentration becomes elevated at several points in the day as the troughs become less well defined. This compounded effect is produced when the flow periods are of insufficient length to completely draw the lead saturated water through the tap. Consequently, high concentrations of lead will remain in the water standing within the lead and copper pipework at the start of the stagnation period. The subsequent stagnation period will thus elevate concentrations further.

The compound effect can be illustrated more clearly by the solution obtained using the plug flow - exponential model for *50m* lead pipework as opposed to *10m* lead pipework (Figure 2.29). In this case, the lead saturated water can only be flushed from the pipework if the flow period is greater than approximately one minute. Consequently, when flow periods are smaller than one minute, a compounded effect is produced. A standard compound effect is witnessed after approximately *100l* of water has been drawn; the subsequent peaks of *50µg/l* represent water that had been standing in the lead pipework for two separate stagnation periods. Similarly, peaks at *68µg/l* and *83µg/l* represent water that had been standing in the lead pipework for three and four separate stagnation periods, respectively.

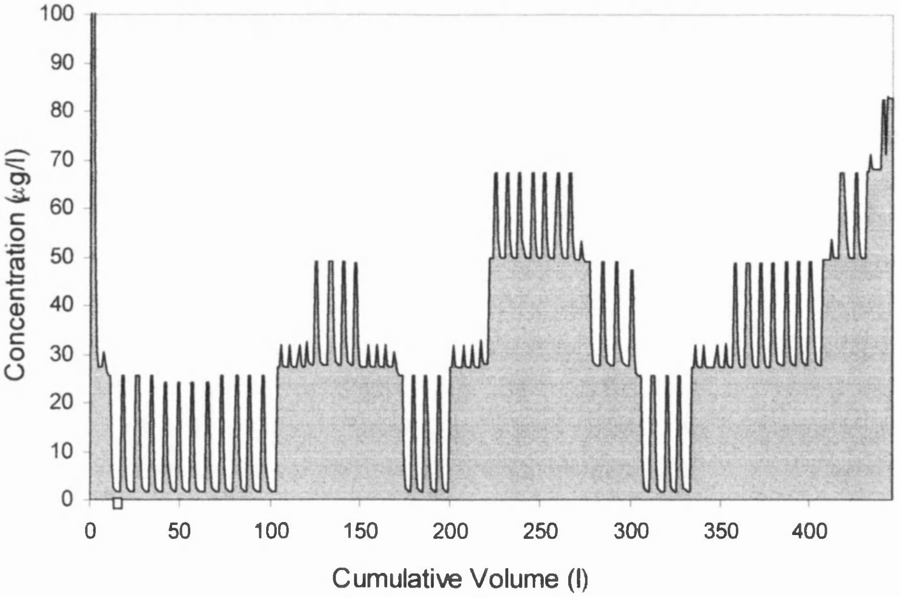


Figure 2.29. Daily concentration variation (50m lead) using plug flow.

The solutions discussed within this subchapter provide a high level of detail in terms of how the concentration at the tap varies for every point during the day for which water is being drawn. Variations throughout individual flow periods have illustrated the peak and trough characteristics of concentration, as well as the possible compound effect. However, in practical terms, the concentration variation throughout a simulated day may be obtained simply by plotting the average concentration at the tap for each flow period (Figure 2.30).

While this solution may not provide the high level of detail previously obtained, it does provides a more realistic representation of the likely concentration of lead found in a typical quantity of water, e.g. a glass of water, drawn from the tap. Although the individual peak and trough behaviour of individual flow events is not characterized, the underlying shape of Figure 2.30 is similar to that of Figure 2.29.

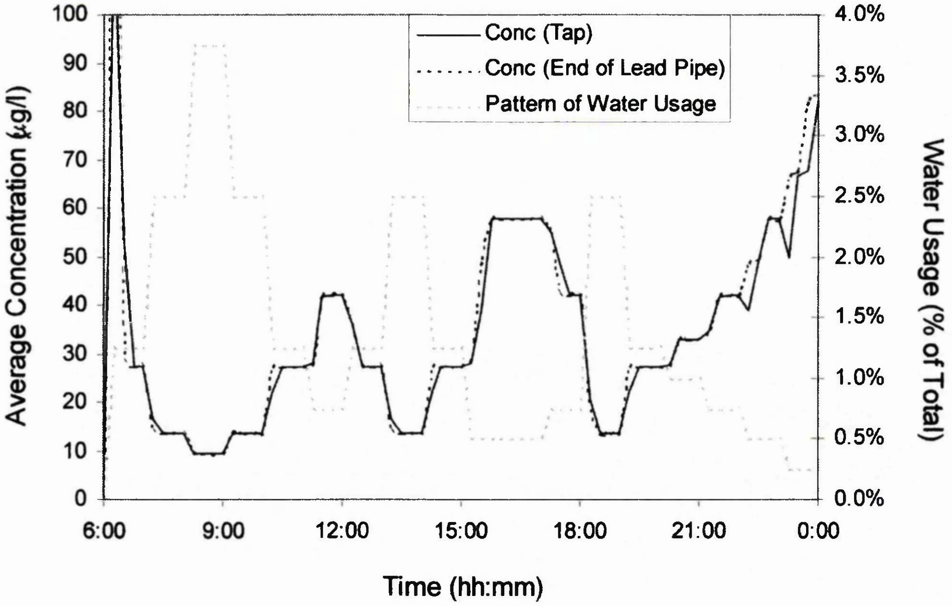


Figure 2.30. Average concentration (50m lead) using plug flow.

The applied pattern of water usage has been superimposed onto this solution revealing its influence on the average concentration during flow. This clearly illustrates that for periods of low water usage, which result in shorter flow periods, the average concentration during flow increases, revealing the compound effect previously discussed. Conversely, as the water usage increases, the flow periods become long enough to allow the lead saturated water to be flushed from the pipework, thus the average concentration decreases to a minimum.

2.4 Sensitivity Analyses

2.4.1 Validation of the single house model

The parameters that influence lead emissions at a single property must be investigated in order to understand the general issues that relate to plumbosolvency control. The most appropriate method of quantifying the extent of the lead emissions occurring at a single property is to compute the daily average concentration (*DAC*) of lead in drinking water that is drawn from the tap, using Eqn. 2.70. This allows a single property to be evaluated with respect to lead emissions in accordance with the new "drinking water" directive since the *DAC* is also representative of a weekly average value ingested by consumers.

However, in order for the single house model to be confidently employed for investigating the influence of household parameters on lead emissions, validation of the model output must be demonstrated for a range of different households. This can be achieved by comparing model results to those obtained from published composite proportional (COMP) sampling data from actual COMP sampling surveys [22]. COMP sampling is arguably the most accurate technique for the measurement of weekly average concentration of lead ingested by consumers at a single property and involves the installation of a sampling device that connects to the kitchen tap as previously described (1.1.9.1.1).

The published COMP survey data [22] includes the COMP sample result (the weekly average concentration of lead) as well as basic household parameters, including length of lead pipework and the number and age of occupants for each household within the survey. A total of 12 different households have been chosen from the survey data so as to include a wide range of different household parameters. The parameters of each chosen house must be input into the model; though parameters that are not explicitly known or reported must be estimated or assumed as follows:

Pipework (internal diameter): *12mm*
Volumetric flow rate, Q: *0.1l/sec*
Daily water consumption: *120l per person per day*
Water usage pattern: *7.5-minute frequency* – 5 or more occupants
15-minute frequency – 2 to 4 occupants
30-minute frequency – 1 occupant
Diffusion coefficient, D: $4.96E\text{-}10 m^2/s$

- Households 1 to 6

  Moderate plumbosolvency, however a cursory analysis of COMP, 30MS and RDT sample concentrations suggest $E > 150$, consequently, the following parameters have been chosen:

  Equilibrium concentration, E: $200\mu g/l$

  Initial mass transfer rate, M: $0.13\mu g/m^2/s$

- Households 7 to 12

  High plumbosolvency, consequently, the following parameters have been chosen:

  Equilibrium concentration, E: $300\mu g/l$

  Initial mass transfer rate, M: $0.2\mu g/m^2/s$

The input data for each household is summarised (Table 2.1). A daily average simulation can be carried out for each household in order to compute the daily average concentration (*DAC*) of lead in drinking water that is drawn from the tap, using Eqn. 2.70. It is likely that the flow within a pipe for typical residential use is turbulent, since the flow rate is approximately *0.1l/s* under normal use, which translates to a Reynolds number greater than *9000*. Consequently, solutions will be obtained from the model for turbulent flow. These will be compared to the equivalent solutions from the more simplistic plug flow model. In the case of the turbulent flow model, solutions will be obtained using the more sophisticated diffusion model. However, in the case of the plug flow model, only the exponential approximation will be used.

Table 2.1. Household Properties.

House ID	M $(\mu g/m^2/sec)$	E $(\mu g/l)$	Pb Length *(m)*	Daily Water Consumption *(l)*
1	0.13	200	10	240
2	0.13	200	18	360
3	0.13	200	41	360
4	0.13	200	27	360
5	0.13	200	35	120
6	0.13	200	10	480
7	0.2	300	3	120
8	0.2	300	12.7	240
9	0.2	300	6.5	120
10	0.2	300	6.3	120
11	0.2	300	9	240
12	0.2	300	5	600

The results illustrate that the model predictions, in terms of *DAC*, for both the plug flow and the more complex turbulent-diffusion model are generally close to the actual COMP sample concentration (Figure 2.31). Notable exceptions to this are houses *7* and *9*, where the model significantly over-estimates and under-estimates the daily average lead emissions, respectively. Such discrepancies may be a result of atypical water consumption, presence of particulate lead or inconsistent operation of the COMP sampling device.

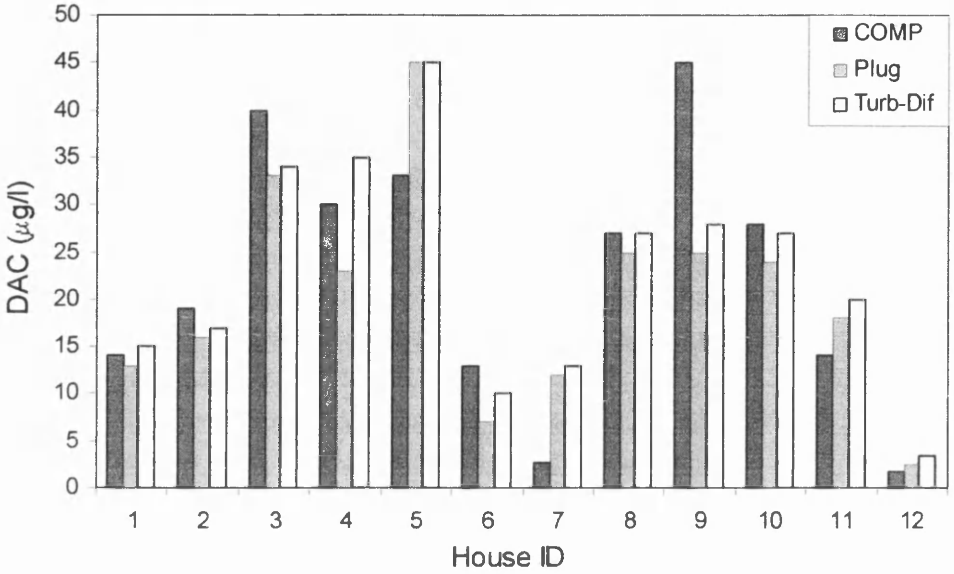


Figure 2.31. Validation of simulated DAC against COMP sample concentrations.

It is concluded that validation has been achieved for a wide range of different household circumstances; consequently the single house model can be confidently employed for investigating the influence of household factors on lead emissions.

2.4.2 Effect of input parameters on daily average concentration

The parameters for a single house that will affect the *DAC*, and therefore must be investigated, are the geometry of the pipework, the water usage and the plumbosolvency of the water:

- Plumbosolvency parameters (*M* and *E* or *D* and *E*)
- Length of lead pipework
- Length of copper pipework
- Diameter of pipework
- Daily water consumption
- Water usage pattern (inter-use time)

- Flow rate

The influence of each parameter on *DAC* can be examined simply by altering one parameter at a time, over a suitable range. The fixed parameters in each case are representative of those that may occur at a typical property having lead pipework and are given the following values:

Pipework (internal diameter):	*12mm*
Pipework (length of lead):	*10m*
Pipework (length of copper):	*0m*
Equilibrium concentration, *E*:	$150\mu g/l$
Initial mass transfer rate, *M*:	$0.1\mu g/m^2/s$
Diffusion coefficient, *D*:	$4.96E\text{-}10m^2/s$
Volumetric flow rate, *Q*:	*0.1l/s*
Daily water consumption:	*450l*
Water usage pattern:	*15-minute frequency*

It is likely that the flow within a pipe for typical residential use is turbulent, since the flow rate is approximately *0.1l/s* under normal use, which translates to a Reynolds number greater than *9000*. Consequently, solutions will be obtained from the model for turbulent flow. However, in order to investigate the influence of flow rate on *DAC*, solutions will be obtained using the laminar flow model when the flow rate is less than *0.05l/s*, which equates to a Reynolds number smaller than *5000*. These solutions will be compared to the equivalent solutions from the simpler plug flow model. In the case of the turbulent flow model, solutions from both diffusion model and exponential approximation of mass transfer can be obtained. However, in the case of the plug flow model, only the exponential approximation will be used.

2.4.2.1 Plumbosolvency

DAC increases linearly with the plumbosolvency of the water for both plug flow and turbulent flow models (Figure 2.32). This linear relationship is in accordance with Eqn. 2.41 and Eqn. 2.54 for the diffusion model and the exponential approximation respectively.

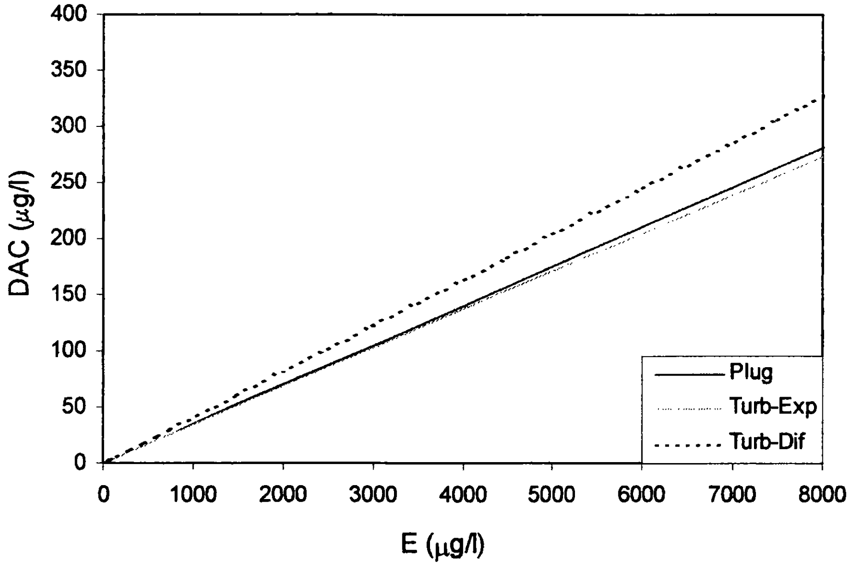


Figure 2.32. Effect of plumbosolvency on DAC.

However, when the diffusion model is used, *DAC* increases at a slightly higher rate. This discrepancy is primarily caused by the subtle differences between the mass transfer models used, i.e. differences between the shapes of the stagnation curves for the exponential model and the diffusion model. In particular, the rate of lead dissolution in the case of the exponential model is lower for stagnation times less than *30* minutes. Since the mean inter-use stagnation time, during the daytime, has been set to *15* minutes, if follows that the exponential approximation underestimate daily lead emissions.

2.4.2.2 Length of lead pipework

The effect of the length of lead pipework on *DAC* is illustrated (Figure 2.33). This shows that *DAC* increases with lead pipe length, essentially a linear relationship up to lengths of about *100m*, the maximum normally encountered. However, for completeness *DAC* has been plotted for lead pipework lengths up to *2000m*.

The initial linear response is expected since the volume of water that is in contact with lead pipework, at any one point in time, increases linearly with length of lead pipework. Additionally, as the length of pipework increases, the flow duration required to flush water standing in the lead pipework increases. For greater lengths of pipework, the typical flow duration is no longer sufficient to flush water from the pipework. Consequently, a proportion of the water supplied will have stood in the pipework for two or more stagnations, producing the compound effect previously discussed (Chapter 2.3.3), thus elevating *DAC* further.

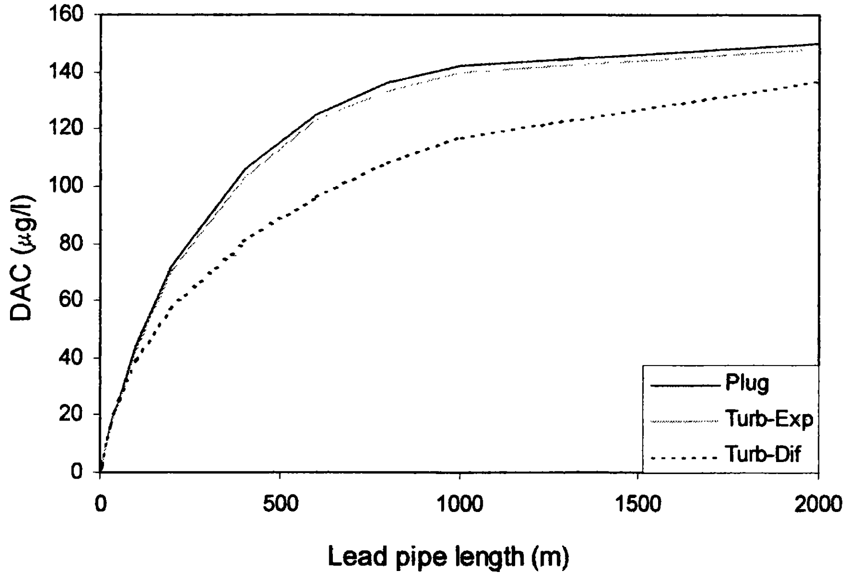


Figure 2.33. Effect of lead pipework length on DAC.

However, as the length of pipework becomes very high, *DAC* begins to exhibit a more logarithmic increase. This is because the concentration increase within the lead pipe is dependant on the difference between the current concentration and the equilibrium concentration *E* in accordance with Eqn. 2.41 and Eqn. 2.54 for the diffusion model and the exponential approximation respectively. Thus, the concentration, and therefore *DAC*, tends to *E* in approximately the same manner as the corresponding stagnation curve.

When the diffusion model is used, the rate of lead dissolution is lower than that for the exponential model for stagnation times greater than *30* minutes (Chapter 2.3.1.3). Consequently, for pipework of lengths greater than *100m*, where the compound effect occurs, *DAC* increases at a slower rate.

2.4.2.3 Length of copper pipework

The effect of the length of copper pipework on *DAC* is illustrated (Figure 2.34). This shows that *DAC* decreases with the length of copper pipework from a maximum value of *5.2µg/l* (exponential approximation) and *6.1µg/l* (diffusion model) for no copper pipework. The effect is negligible, with a *1%* decrease in *DAC* observed for a *10m* length of copper pipework, and a *15%* decrease in *DAC* observed for a *200m* length of copper pipework.

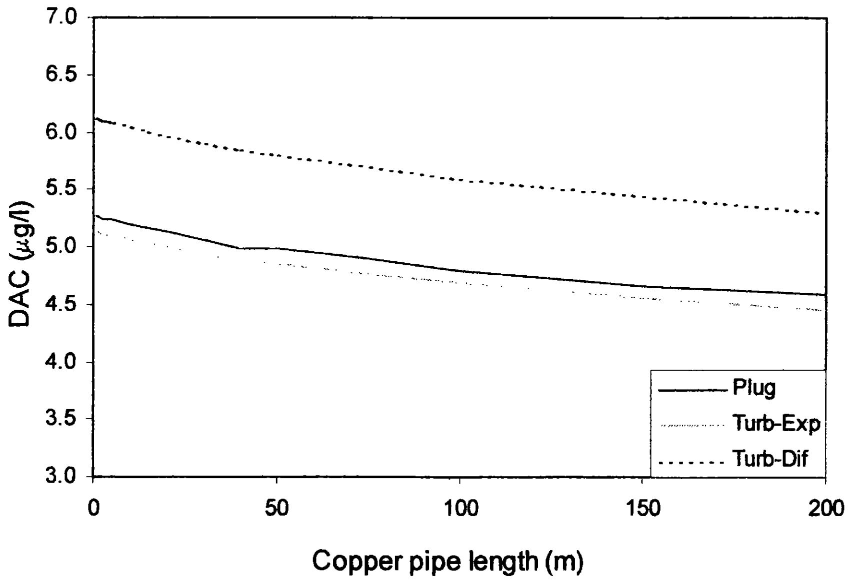


Figure 2.34. Effect of copper pipework length on DAC.

This decrease in *DAC* is caused by the fact that an increasing quantity of lead remains in the pipework at the end of the simulated day since the final flow period is of insufficient duration to flush this from the pipework. Consequently, the remaining lead does not get to the tap, and therefore does not contribute to *DAC*. This phenomenon is a consequence of setting the initial concentration within the pipework to zero at the start of the simulated day. However, by setting the initial concentration within the pipework to the 'end of day' concentrations, thus emulating the real world more closely, the conservation of mass is maintained and copper pipe length does not effect *DAC*.

Once again, *DAC* is consistently higher for the diffusion model since the rate of lead dissolution is greater for stagnation times less than *30* minutes.

2.4.2.4 Diameter of pipework

In the case of the exponential model, *DAC* effectively increases linearly with pipework diameter. (Figure 2.35), though the actual relationship is actually logarithmic with *DAC* tending to *E*. This is because the surface area in contact with the given daily volume of water flowing through the lead pipe is greater. Since concentration is uniform across the entire pipe cross-section for the exponential approximation, it follows from Eqn. 2.54 that concentration, and therefore *DAC*, increases with surface area.

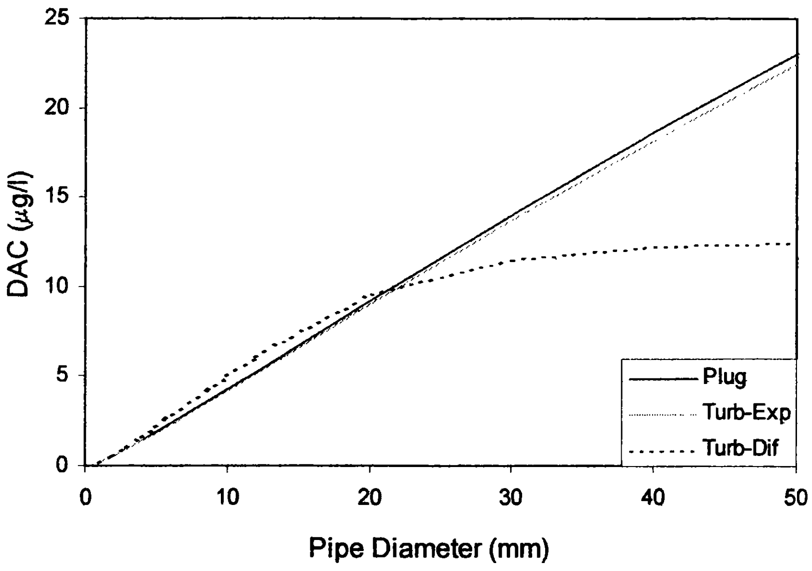


Figure 2.35. Effect of pipework diameter on DAC.

In the case of the diffusion model, the lead enters the water from the pipe wall and so the concentration in the centre of the pipe remains low for small durations of stagnation as previously illustrated (Figure 2.15). This effect becomes more apparent as diameter increases and it is found that the average concentration of water standing within the lead pipework decreases. However, the proportion of the given daily volume of water that stagnates within the lead pipework increases linearly with diameter. These two effects combine and produce the logarithmic relationship observed (Figure 2.35).

2.4.2.5 Daily water consumption

In the case of both exponential and diffusion model, *DAC* decreases with increasing daily water consumption, the relationship being logarithmic (Figure 2.36). As water consumption decreases, the average flow duration must also decrease assuming a fixed inter-use time. Consequently, water that is eventually supplied will have stood in the pipework for increasing lengths of time, producing the compound effect previously discussed (Chapter 2.3.3), thus elevating *DAC* further.

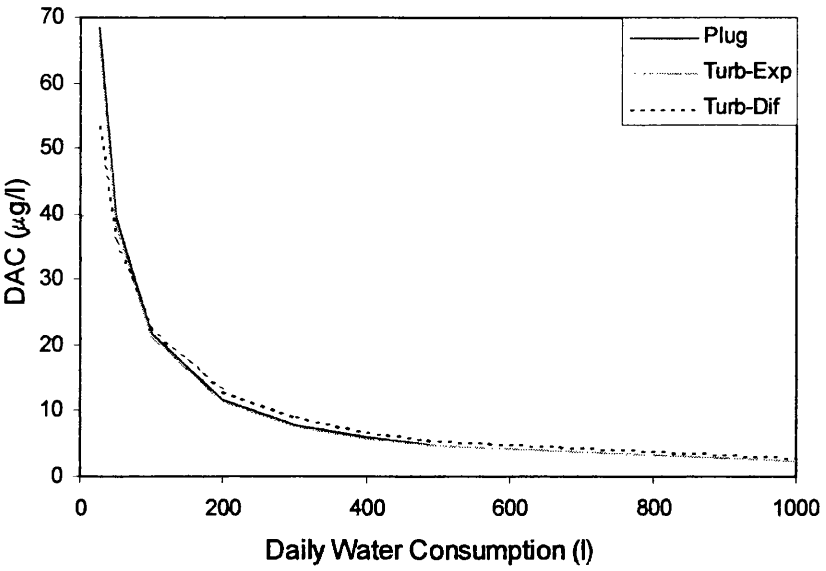


Figure 2.36. Effect of daily water consumption on DAC.

Conversely, when water consumption increases, the average flow duration must also increase assuming a fixed inter-use time. Consequently, each period of flow will be of sufficient duration to completely flush the pipework of water that had previously been stagnating and the compound effect will not be observed. Additionally, as the water consumption, and therefore flow duration, is increased, the stagnation time decreases. Thus, in the most extreme case the tap will be open for the entire *24 hour* period and the resulting *DAC* will be representative of the steady state concentration.

2.4.2.6 Inter-use time

Inter-use time is simply the duration between successive water usage events, defining the frequency with which water is used at a house. In the case of both exponential and diffusion model, *DAC* decreases with increasing inter-use time (Figure 2.37). This is because, for a given daily volume, more water stagnates in the lead pipework when the mass transfer rate is at its highest, i.e. at the start of the stagnation curve. In the case of the exponential model, the stagnation curve is effectively linear during the first hour. Consequently the concentration and therefore *DAC* decreases linearly with inter-use time.

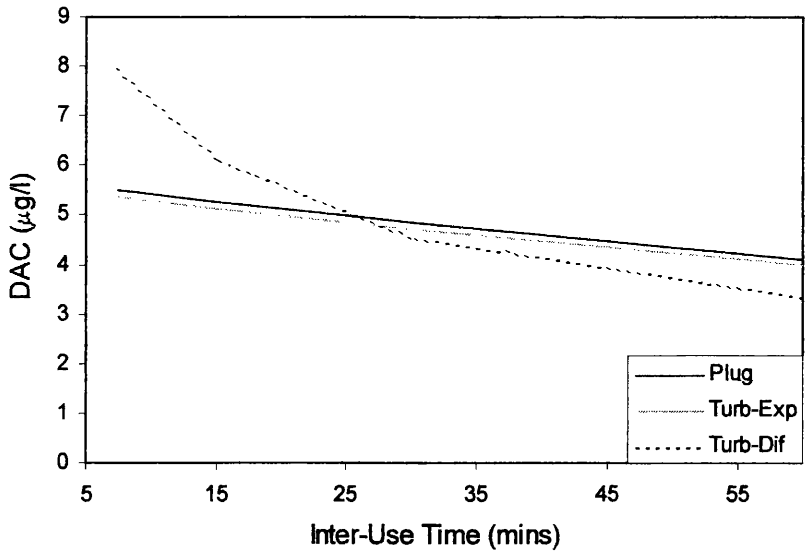


Figure 2.37. Effect of inter-use time on DAC.

The influence of inter-use time is significantly greater for the diffusion model, specifically revealing markedly higher *DAC* for small inter-use times. This is because the rate of lead dissolution in the case of the diffusion model is considerably higher than that for the exponential model for shorter stagnation times, resulting in higher concentrations and therefore higher *DAC*. Conversely, the rate of lead dissolution in the case of the diffusion model is lower than that for the exponential model for stagnation times greater than *30* minutes, thus *DAC* is lower.

Note that since the exponential and diffusion models are both calibrated to the same *30*-minute data point, the *DAC* for an inter-use time of *30* minutes are virtually the same.

2.4.2.7 Flow rate

In the case of both exponential and diffusion model, *DAC* decreases with increasing flow rate (Figure 2.38). This is because the water is in contact with the lead pipework for a greater duration when the flow rate is low. Additionally, when the flow rate is very low, the duration of the flow events must increase for fixed daily water consumption. Consequently, *DAC* becomes more representative of the steady state concentration, which increases as the flow rate decreases. However, the influence on *DAC* is only significant at low flow rates; no further effect being observed for flow rates greater *0.5l/s* (Figure 2.39).

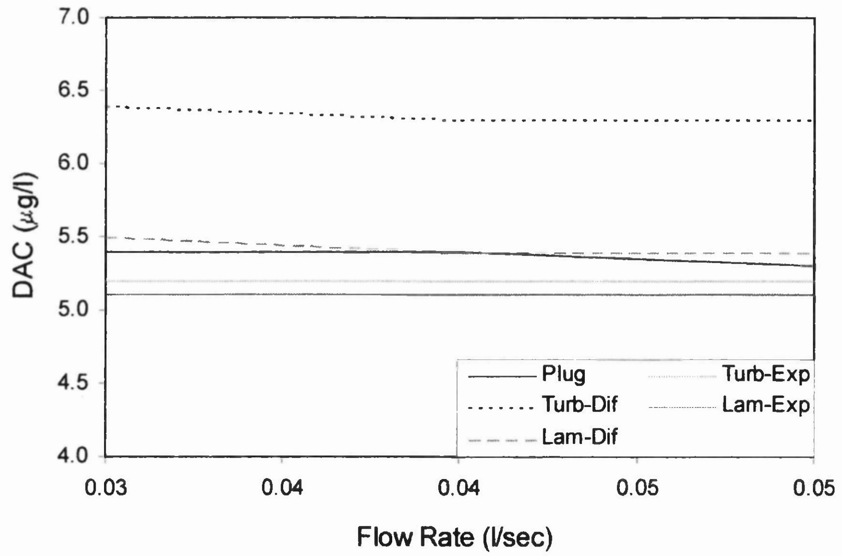


Figure 2.38. Effect of flow rate (low) on DAC.

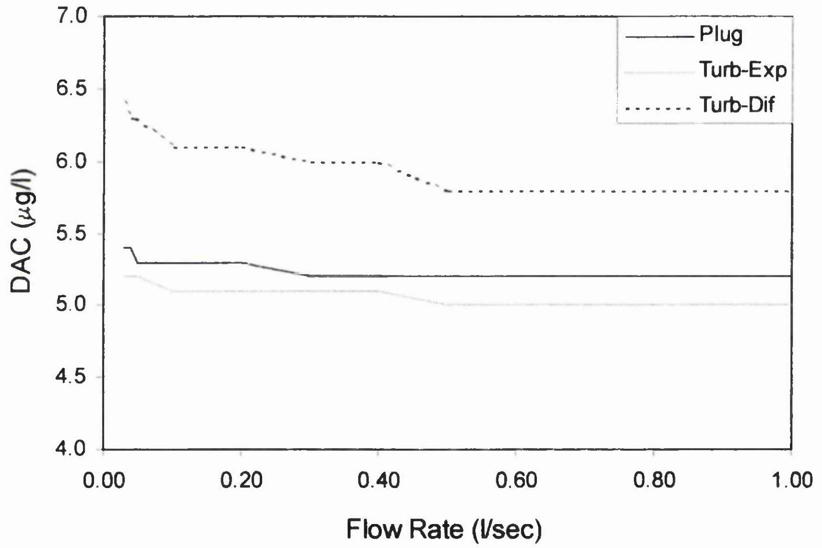


Figure 2.39. Effect of flow rate (high) on DAC.

2.4.3 Effect of input parameters on 30MS

In addition to *DAC*, it is possible to model the standard "30-minute stagnation" test, widely used in the UK for benchmarking the success of plumbosolvency control treatment. Consequently, in order to investigate the effect of parameters, such as pipework and water usage, on lead emissions at a single property, both *DAC* and the "30-minute stagnation" test result (*30MS*) will be employed for the characterisation of lead emissions.

The "30-minute stagnation" test sample, having volume *1.0 litre*, is taken at approximately *0.1l/s* from the tap after a fixed stagnation period, which commences after the pipework has been fully flushed. Consequently, it is logical to assume that the parameters that relate to water usage, such as the pattern of water usage and the daily water consumption, will not affect the *30MS* and can be ignored. The remaining parameters that will affect the *30MS* and must be investigated are the geometry of the pipework and the plumbosolvency of the water:

- Plumbosolvency parameters (M and E or D and E)
- Length of lead pipework
- Length of copper pipework
- Diameter of pipework

The influence of each parameter on *30MS* can be examined simply by altering one parameter at a time, over a suitable range. The fixed parameters in each case are representative of those that may occur at a typical property having lead pipework and are given the following values:

Pipework (internal diameter):	*12mm*
Pipework (length of lead):	*10m*
Pipework (length of copper):	*0m*
Equilibrium concentration, E:	*150µg/l*
Initial mass transfer rate, M:	$0.1 \mu g/m^2/s$
Diffusion coefficient, D:	$4.96E\text{-}10 m^2/s$
Volumetric flow rate, Q:	*0.1l/sec*
Daily water consumption:	*450l*
Water usage pattern:	*15-minute frequency*

It is likely that the flow within a pipe for typical residential use is turbulent, since the flow rate is approximately *0.1l/s* under normal use, which translates to a Reynolds number greater than *9000*. Consequently, solutions will be obtained from the model for turbulent flow. These will be compared to the equivalent solutions from the simpler plug flow model. In the case of the turbulent flow model, solutions from both diffusion model and exponential approximation of mass transfer can be obtained. However, in the case of the plug flow model, only the exponential approximation will be used.

2.4.3.1 Plumbosolvency

The plumbosolvency of the water is defined by factors M and E (exponential model) and factors D and E (diffusion model). An increase in plumbosolvency is characterised by an increase in solubility *E*. However, in the case of the exponential approximation, it is also necessary to increase the initial mass transfer rate, *M* by the same proportion.

The effect of plumbosolvency on *30MS* is illustrated (Figure 2.40). Clearly, *30MS* increases in direct proportion to the plumbosolvency of the water for both plug flow and turbulent flow models. This response is expected since, in the absence of copper pipework, *30MS* is approximately equal to the concentration in the lead pipework after a *30-minute* stagnation. This increases with plumbosolvency is in accordance with Eqn. 2.41 and Eqn. 2.54 for the diffusion model and the exponential approximation respectively.

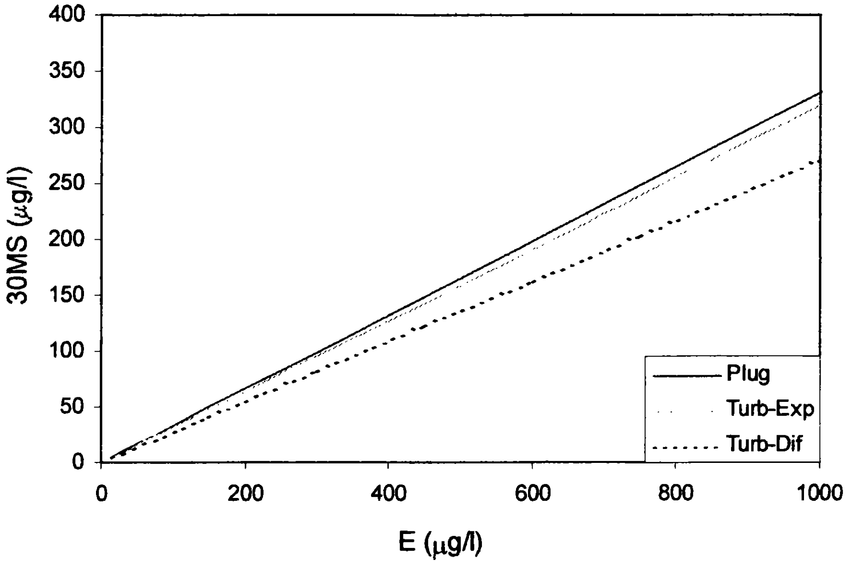


Figure 2.40. Effect of plumbosolvency on 30MS.

However, when the diffusion model is used, the increase in *30MS* is noticeably lower. This discrepancy can be explained by considering how the concentration varies across the pipe cross-section for each model for mass transfer during stagnation. After short stagnation periods, e.g. *30 minutes*, the concentration, computed using the diffusion model, is highest near to the pipe wall, diminishing to virtually zero in the centre of the pipe. However, in the case of turbulent flow, the velocity close to the pipe wall is lowest, consequently the volume averaged concentration at the tap will be lower when using the diffusion model.

2.4.3.2 Length of lead pipework

The effect of the length of lead pipework on *30MS* is illustrated (Figure 2.41). This shows that *30MS* effectively increases in direct proportion to the length of lead pipework, from zero to up to a maximum value of approximately *50μg/l* (exponential approximation) and *40µg/l* (diffusion model), after which *30MS* remains constant for increasing lead pipework length.

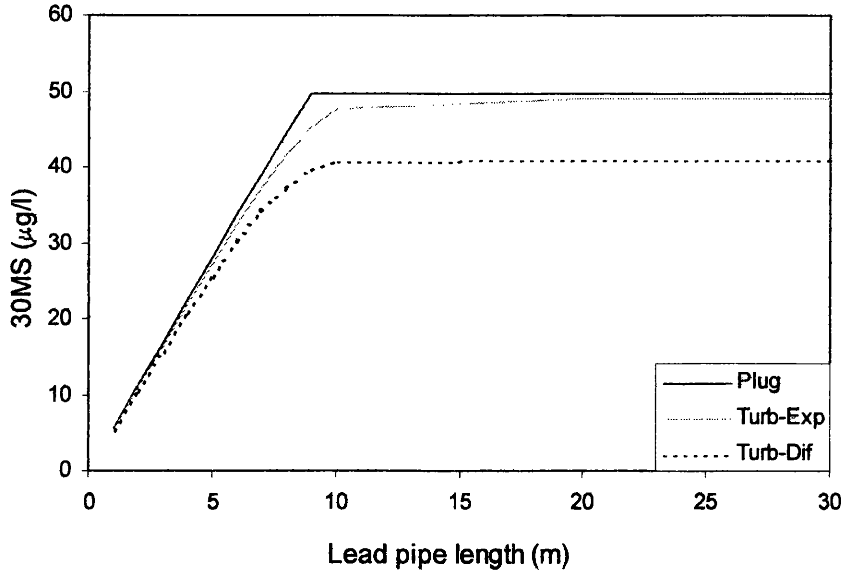


Figure 2.41. Effect of lead pipework length on 30MS.

The initial linear response is expected since the *1-litre* sample, taken at the tap, will be comprised of water that has stagnated in the lead pipework, which will thus contain lead, as well as fresh water from the water main, which will not contain lead. The proportion of water that has stagnated in the lead pipework is proportional to the length of lead pipework, thus determining the *30MS* obtained. However, in the case of plug-flow, when the volume of the lead pipework exceeds *1.0 litre*, i.e. the length of the pipework exceeds *9m*, the *1-litre* sample will only be comprised of water that has stagnated in the lead pipework and the dilution effect will not be observed. Consequently, the *30MS* obtained is equal to the concentration in the lead pipework after a *30-minute* stagnation, i.e. a maximum of *50µg/l*. In the case of turbulent flow, the peak concentration is not obtained until a pipework length of *10m* since the velocity profile causes the flow in the centre of the pipe to move faster, resulting in the flushing effect occurring below *10m*.

Note also that when the diffusion model is used, the peak *30MS* is noticeably lower. This discrepancy can be explained by considering how the concentration varies across the pipe cross-section for each model of mass transfer during stagnation, as previously described.

2.4.3.3 Length of copper pipework

The effect of the length of copper pipework on *30MS* is illustrated (Figure 2.42). This shows that *30MS* effectively decreases in direct proportion to the length of copper pipework from a maximum value of *50μg/l* (exponential approximation) and *40μg/l* (diffusion model) for no copper pipework, to zero at *9m* or more copper pipework.

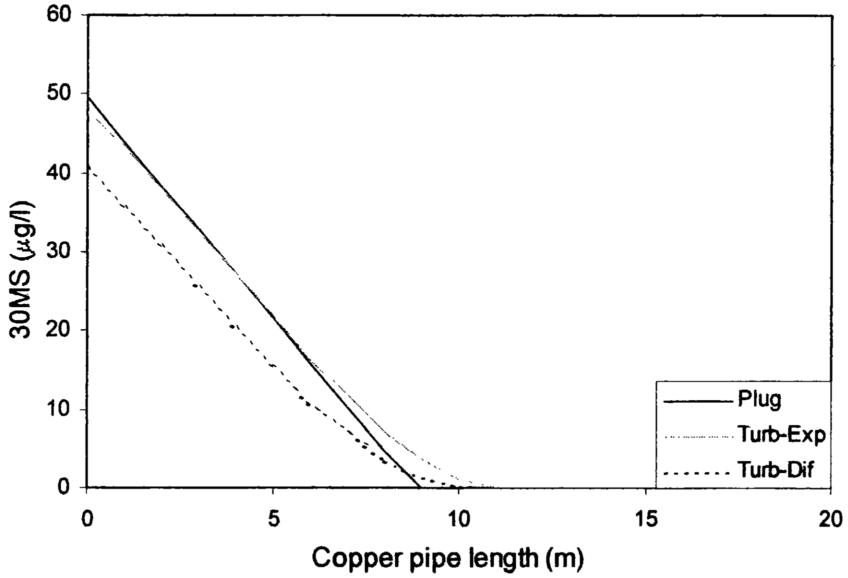


Figure 2.42. Effect of copper pipework length on 30MS.

As before, the initial linear response is expected since the *1-litre* sample, taken at the tap, will be comprised of water that has stagnated in the lead pipework, which will thus contain lead, as well as water that has stagnated within the copper pipework, which will not contain lead. The proportion of water that has stagnated in the copper pipework is proportional to the length of copper pipework, thus determining the *30MS* obtained. However, in the case of plug-flow, when the volume of the copper pipework exceeds *1.0 litre*, i.e. the length of the pipework exceeds *9m*, the *1-litre* sample will only be comprised of water that has stagnated in the copper pipework. Consequently, the *30MS* obtained is equal to the concentration in the copper pipework after a *30-minute* stagnation, i.e. zero, since there is no source of lead here. In the case of turbulent flow, the peak concentration is not obtained until a pipework length of *10m* since the velocity profile causes the flow in the centre of the pipe to move faster, resulting in lead from the lead pipework reaching the tap when the length of the copper pipework is less than *10m.*

Note also that the peak *30MS*, occurring at *0m* copper pipework, is equal to the peak *30MS* obtained in Chapter 2.4.3.2. Consequently, this discrepancy can be explained in exactly the same manner.

2.4.3.4 Diameter of pipework

The effect of pipework diameter on *30MS* is illustrated (Figure 2.43). This shows that *30MS* effectively increases in direct proportion to the diameter of pipework from zero to a maximum value of *50μg/l* (exponential approximation) and *40μg/l* (diffusion model) at a diameter of approximately *12mm*. For diameters greater than *12mm*, *30MS* decreases logarithmically with increasing diameter.

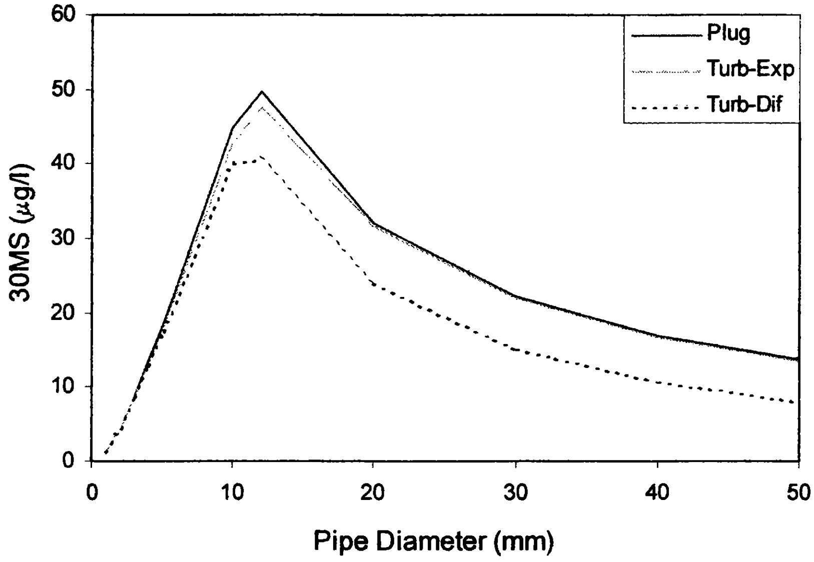


Figure 2.43. Effect of pipework diameter on 30MS.

When the volume of the lead pipe is greater than *1.0 litre*, the *30MS* obtained is equal to the concentration in the lead pipework after a *30-minute* stagnation, which decreases with increasing pipework diameter due to the lower surface area to volume ratio. This is in accordance with Eqn. 2.41 and Eqn. 2.54 for the diffusion model and the exponential approximation respectively. Consequently, a logarithmic decline in *30MS* is observed for pipework diameter greater than *12mm*, which corresponds to a volume greater than *1.0 litre*.

However, when the pipework diameter is reduced from *12mm*, the volume of the lead pipework also reduces, consequently the *30MS* obtained will be a function of both the diameter effect, discussed above, as well as the dilution effect, discussed previously. The dilution effect quickly becomes dominant since pipework volume decreases with the square of pipework diameter.

Once again, when the diffusion model is used, the peak *30MS* is noticeably lower. This discrepancy can be explained by considering how the concentration varies across the pipe cross-section for each model of mass transfer during stagnation, as previously described.

It is possible to remove the dilution effect completely in order to investigate the diameter effect alone simply by increasing the length of lead pipework appropriately. The corresponding solutions illustrate how *30MS* decreases logarithmically with increasing pipework diameter over the entire range of diameter (Figure 2.44). Through extrapolation, it is clear that the maximum *30MS*, equal to the equilibrium, occurs at diameters close to *0mm.*

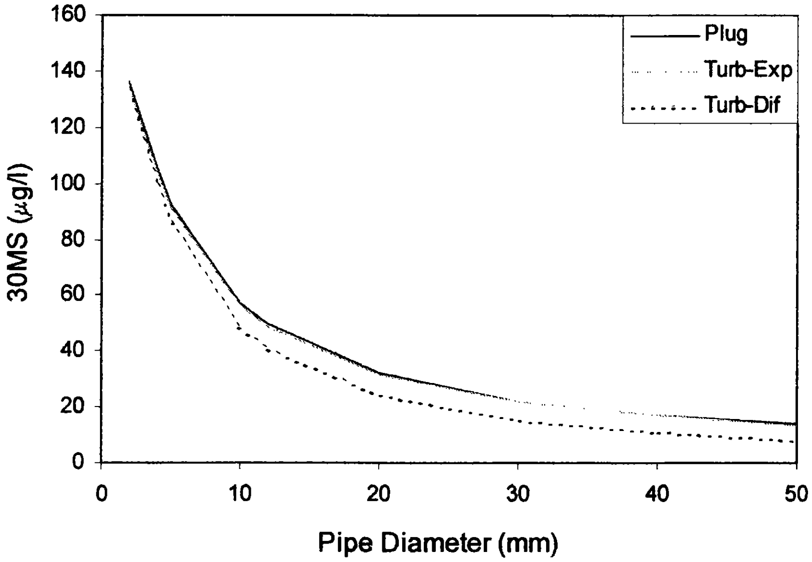


Figure 2.44. Effect of pipework diameter on 30MS (long lead pipework).

2.4.4 Effect of discretisation

In order to model spatial and temporal variations in concentration it has been necessary to discretised the domain, i.e. the pipework, and also discretise the time for which a stagnation or flow period takes place. The pipework is discretised in the axial direction (i, $i = 1, N$), and in the radial direction (j, $j = 1, J$), whilst time is discretised as (t, $t = 1,n$). It is necessary to impose the condition that the volume of water in any axial element cannot be completely emptied in less than one timestep (Eqn. 2.28), as previously discussed. Consequently, the spatial discretisation in the axial direction can be calculated from the temporal discretisation chosen and vice versa.

The application of higher resolutions of discretisation, i.e. smaller increments in space and time, generally result in a more accurate computational model. However, this will increase the computation time considerably; consequently, it is necessary to make a compromise between speed and accuracy.

The resolution of the temporal discretisation was chosen as Δt = *1 second*, for simplicity. For the standard assumptions of $Q = 0.1 l/s$ and $r_o = 6mm$, this timestep resulted in a spatial resolution of $\Delta x = 0.88m$, *1.77m* and *1.08m* for plug-flow, laminar flow and turbulent flow, respectively. In order to accurately represent the rapid variation in velocity in the region next to the pipe wall that occurs under turbulent flow, the number of radial elements was chosen as $J = 40$.

In order to justify the application of this chosen discretisation it is necessary to investigate solutions obtained from the computational model for a range of discretisation resolutions. The influence of the discretisation on various solutions including *DAC*, *30MS* and concentration variation during flow will be examined. These solutions will be obtained using the standard input parameters of a typical property, used previously (Chapter 2.4.2). As before, solutions will be obtained from the model for turbulent flow and from the simpler plug flow model. In the case of the turbulent flow model, solutions from both diffusion model and exponential approximation of mass transfer can be obtained. However, in the case of the plug flow model, only the exponential approximation will be used. Additionally, the plug flow model will only be used to investigate discretisation in the axial direction since it does not apply radial discretisation.

2.4.4.1 Concentration at tap

In the case of the turbulent – diffusion model, the peak volume averaged concentration at tap during flow increases with increasing radial discretisation (Figure 2.45). However, the increase becomes progressively smaller and the solution converges.

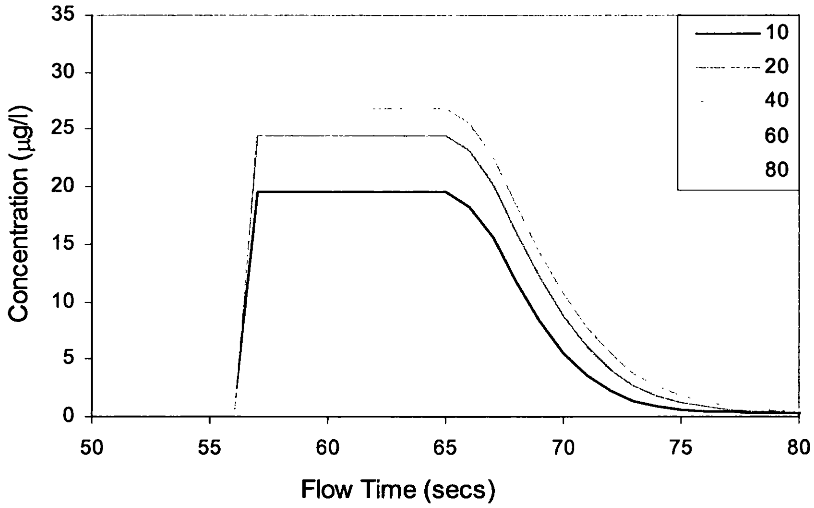


Figure 2.45. Effect of *J* on concentration during flow (turbulent - diffusion).

The computational error at $J = 10$ radial elements is very large at approximately *30%*, while the error at $J = 40$ radial elements is only *3%*, consequently the chosen radial discretisation of $J = 40$ is justified because the error is sufficiently small. A similar result is obtained for the turbulent – exponential model, though the solution converges faster.

The peak volume averaged concentration increases with increasing radial discretisation because the turbulent velocity profile is more accurately represented, in particular the rapid variation in velocity in the region next to the pipe wall. Consequently, the contribution from the region very close to the pipe wall can be more fully accounted for, thus increasing the average concentration. This effect is particularly significant in the case of the diffusion model because the majority of dissolved lead is found in the region very close to the pipe wall.

Conversely, for increasing axial discretisation, the peak volume averaged concentration at tap during flow remains constant (Figure 2.46). This is because, in the case of *10m* lead pipework, the concentration at the end of a stagnation period is effectively the same throughout the entire lead pipework, irrespective of the axial discretisation. Consequently, the volume averaged concentration at the start of the flow period, which is the peak concentration, is the same. However, as the resolution of the axial discretisation is increased, the resolution of the temporal discretisation must also be increases in accordance with (Eqn. 2.28), thus the concentration variation within the lead pipe and the variation over time is better represented.

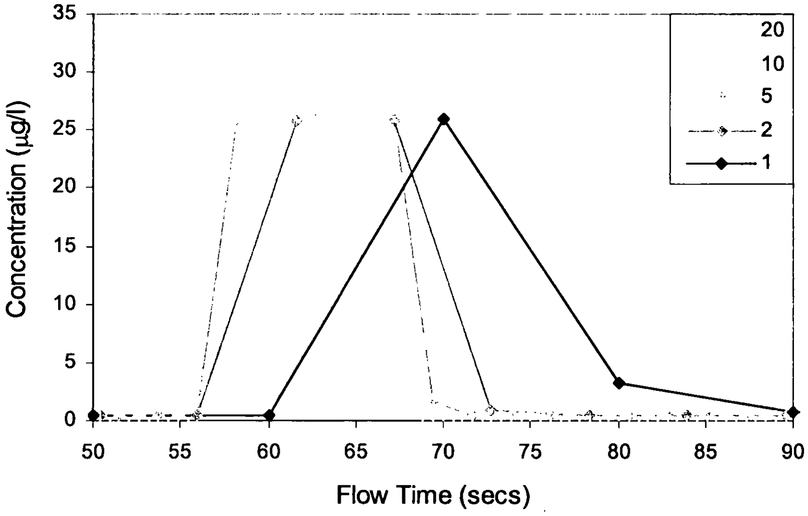


Figure 2.46. Effect of N on concentration during flow (plug).

In the most extreme example, the entire lead pipework is represented using just one axial element ($N = 1$), and the temporal discretisation is $\Delta t = 10$ *sec*. Since it takes approximately *10 sec* for the majority of the lead to be flushed from the lead pipework, the peak concentration is only measured at one timestep (the beginning of the flow period).

2.4.4.2 Daily average concentration

For increasing radial discretisation, the daily averaged concentration (*DAC*) for turbulent flow increases with increasing radial discretisation for both exponential and diffusion models (Figure 2.47). However, the increase becomes progressively smaller and the solution converges in both cases. Thus, the chosen radial discretisation of $J = 40$ is justified because the error is sufficiently small. However, in the case of the exponential model, where the effect of radial discretisation is smaller, a radial discretisation of $J = 20$ would be justified.

The relationship between *DAC* and *J* is a direct result of the effect of radial discretisation on the peak concentration during flow, previously discussed. Once again, this effect is particularly significant in the case of the diffusion model because the majority of dissolved lead is found in the region very close to the pipe wall.

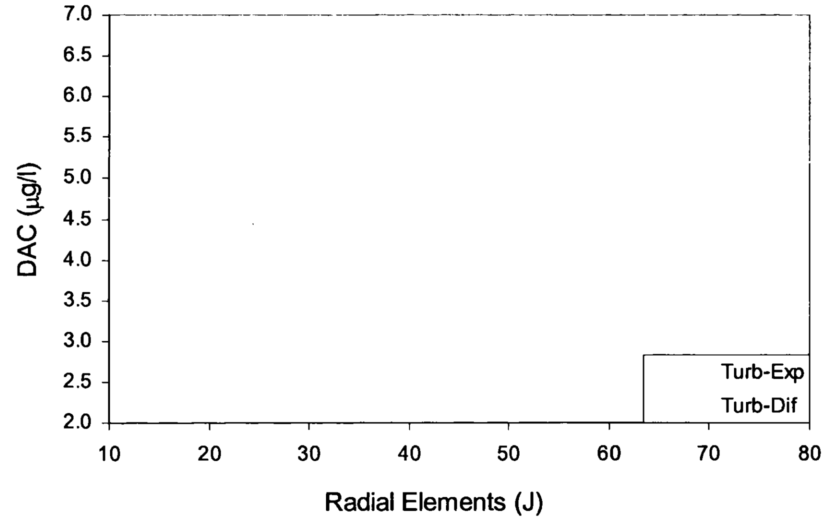


Figure 2.47. Effect of *J* on *DAC* (turbulent flow).

Conversely, for increasing axial discretisation, *DAC* effectively remains constant for plug flow as well as turbulent flow (Figure 2.48). When greater axial discretisation, which results in smaller Δt, is employed, the computational model is capable of representing the immediate concentration variation in space and time more accurately. However, although course discretisation cannot represent this fine detail, it can represent an average concentration for a given flow period. This can be illustrated by the fact that the areas beneath each curve in Figure 2.46, which represents quantity of dissolved lead, are approximately equal, despite difference in the shape of the curves. This is a result of imposing conservation of mass within the model. Consequently, for the purposes of computing *DAC*, the employment of course axial/temporal discretisation (*N = 1, Δt = 10*) is justified.

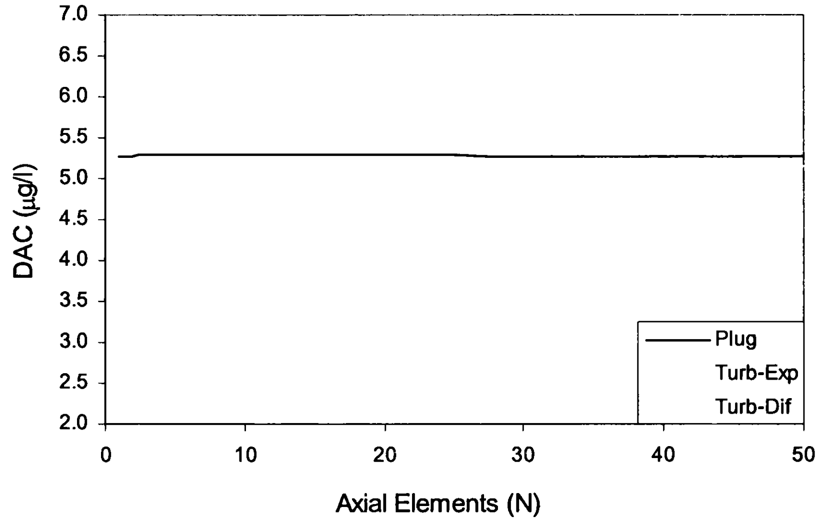


Figure 2.48. Effect of *N* on *DAC*.

2.4.4.3 30 minute stagnation test

For increasing radial discretisation, the "30-minute stagnation" test result (*30MS*) for turbulent flow increases with increasing radial discretisation for both exponential and diffusion models (Figure 2.49). However, the increase becomes progressively smaller and the solution converges in both cases. This relationship is a direct result of the effect of radial discretisation on the peak concentration during flow, previously discussed.

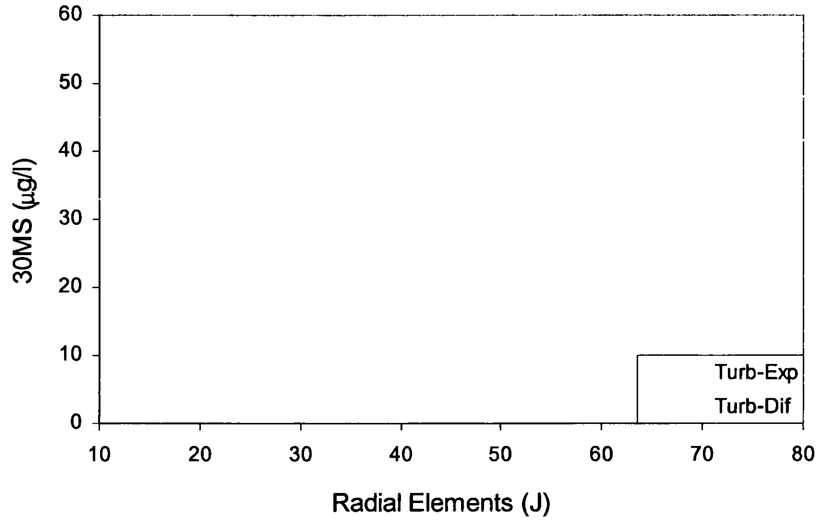


Figure 2.49. Effect of *J* on *30MS* (turbulent flow).

As in the case of *DAC*, the chosen radial discretisation of $J = 40$ is justified because the error is sufficiently small. However, in the case of the exponential model, where the effect of radial discretisation is smaller, a radial discretisation of $J = 20$ would be justified.

Conversely, for increasing axial discretisation, *30MS* effectively remains constant for plug flow as well as turbulent flow (Figure 2.50). As with *DAC*, course discretisation is sufficient to represent the average concentration over a flow period of *10 secs*, required to draw the *1 litre* sample of water.

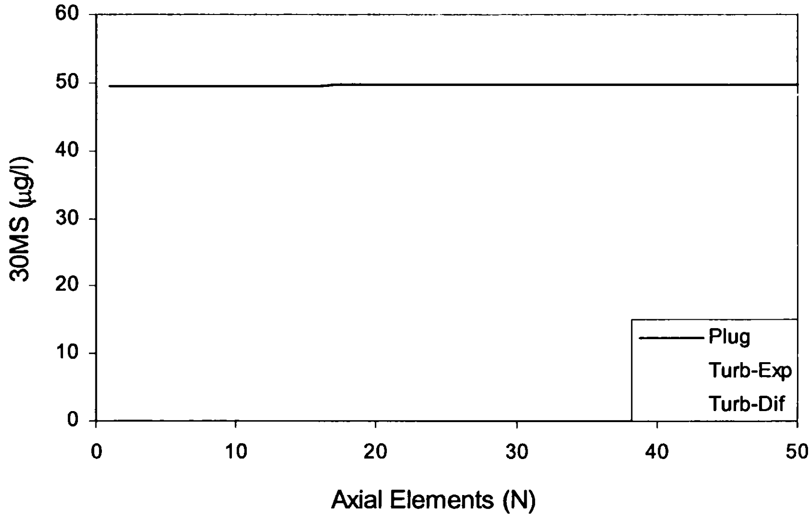


Figure 2.50. Effect of *N* on *30MS*.

2.5 Experimental work

2.5.1 Objectives

Plumbosolvency is characterised by the relationship between lead dissolution and water contact (stagnation) time, which forms the characteristic 'stagnation curve' (Figure 1.3). It has been found that household lead emissions, in terms of a daily average concentration (*DAC*), increase linearly with the plumbosolvency of the water (Chapter 2.4.3.1). Consequently, in order to accurately predict household lead emissions for a particular water, it is necessary to characterise the plumbosolvency characteristics for that water and calibrate the computational model accordingly. In particular, the diffusion coefficient, D (m^2/s) and the equilibrium or solubility concentration, E $(\mu g/l)$ must be obtained in order to calibrate the diffusion model. Additionally, obtaining the actual stagnation curve for a real water will enable the response predicted by the diffusion model to be substantiated.

Solubility of lead in water depends on the composition of the water, in particular the pH, alkalinity, phosphate content as well as temperature. Thus, in order to assess the plumbosolvency of a water, it is also necessary to determine the basic parameters that effect plumbosolvency such as pH and temperature.

2.5.2 Methodology

A lead pipe rig, essentially consisting of three horizontal lead pipes, each of length *5m* and connected to a header tank, was assembled (Figure 2.51). All pipe-work, valves and taps connecting to and from the sections of lead pipe are made of plastic in order to eliminate galvanic corrosion. Temperature sensors connected to a data logger were attached to both header tank and one lead pipe for the purposes of measuring concentration variations throughout the experiment. The purpose of using three separate lead pipes was to obtain triplicate sets of results for each experiment in order to demonstrate reproducibility.

After the rig was hydrologically tested for leaks and cleaned thoroughly the lead pipes underwent conditioning with the testing water. This was carried out by flushing a quantity of the test water through the pipework and allowing the test water to stagnate for *24 hours*; the process being repeated over a two-week period. The purpose of conditioning the pipes was to develop, as far as possible, a stable internal corrosion deposit (scale) that would be present in a lead pipe supplying a real property [74]. The formation of a corrosion deposit, e.g. lead carbonate, on the inner wall of the lead pipe during the conditioning period will lower the solubility of lead in water significantly.

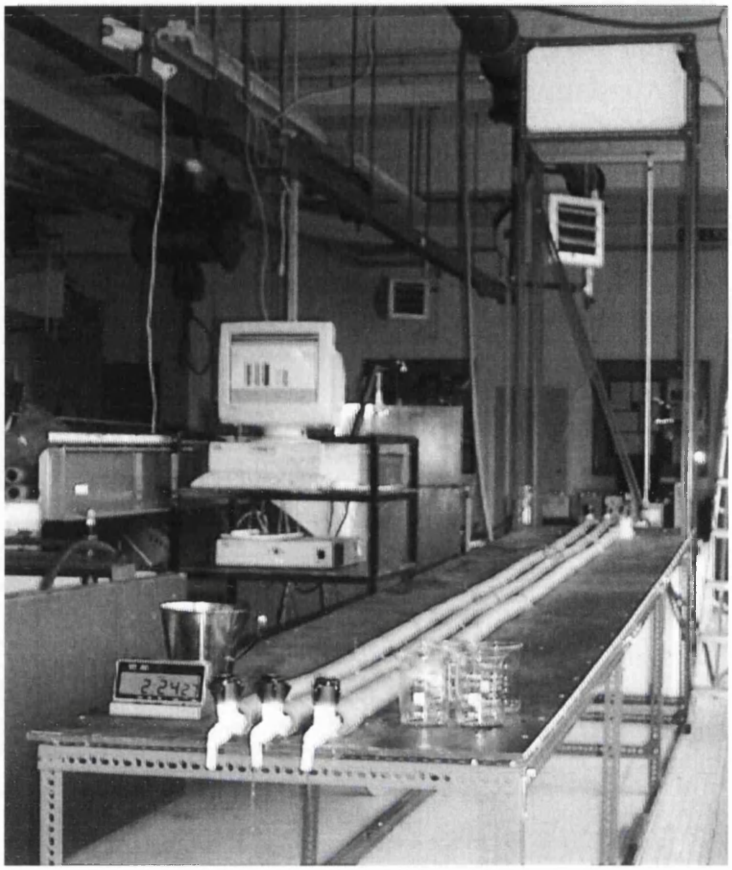


Figure 2.51. Lead pipe rig.

The testing procedure itself involved the collection of *500ml* samples of water from each lead pipe after each controlled stagnation period. Before each stagnation, the lead pipes were flushed with the testing water in order to ensure that the initial concentration of the water within the lead pipes was effectively zero. Additionally, a *500ml* sample of water was taken from the header tank prior to each controlled stagnation period in order to assess the effect of stagnation on the properties of the test water.

Samples were obtained for a range of stagnation times, including several *30-minute* stagnation periods and several very long stagnation periods. The temperature, pH and phosphate content of each sample were measured prior to storage in airtight containers. After samples had been obtained for a sufficient range of stagnation times, they were sent to Severn Trent Laboratories for measurement of dissolved lead content. Temperature data that had been logged for both header tank and lead pipe were analysed and saved for future reference.

2.5.3 Results

Plumbosolvency characteristics for several different testing waters were successfully obtained from the lead pipe rig. Results for two contrasting waters will be illustrated, where:

- Test-Water-A: Phosphated uplands water having low plumbosolvency.
- Test-Water-B: Unphosphated chalk groundwater having moderately plumbosolvency.

Sample concentrations for the "30-minute stagnation" test (*30MS*), which were taken at various times during the conditioning period, are shown for Test-Water-A (Figure 2.52). This illustrates how lead emissions decrease as the corrosion deposit is formed on the inner wall of the fresh lead pipe during conditioning. In this case, the stable corrosion deposit formed is lead phosphate. Consequently, the reduction in solubility during the conditioning period is large since the solubility of lead phosphate is very low. These findings are in direct agreement with those obtained by Colling [38,43], previously illustrated (Figure 1.4).

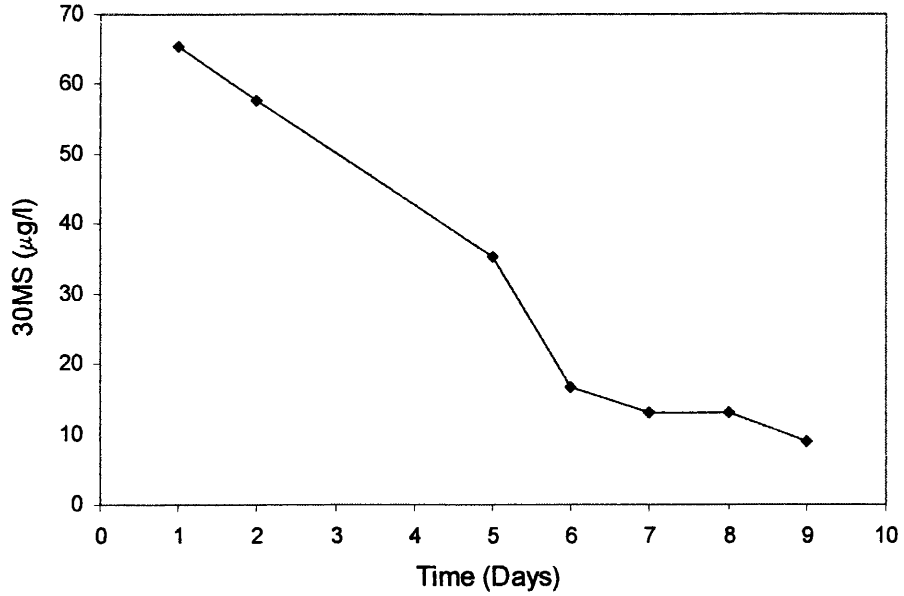


Figure 2.52. 30MS Concentration during the conditioning period.

The principal results from experimental work, based on sample concentrations taken after the conditioning period, are shown for two contrasting waters (Figure 2.53).

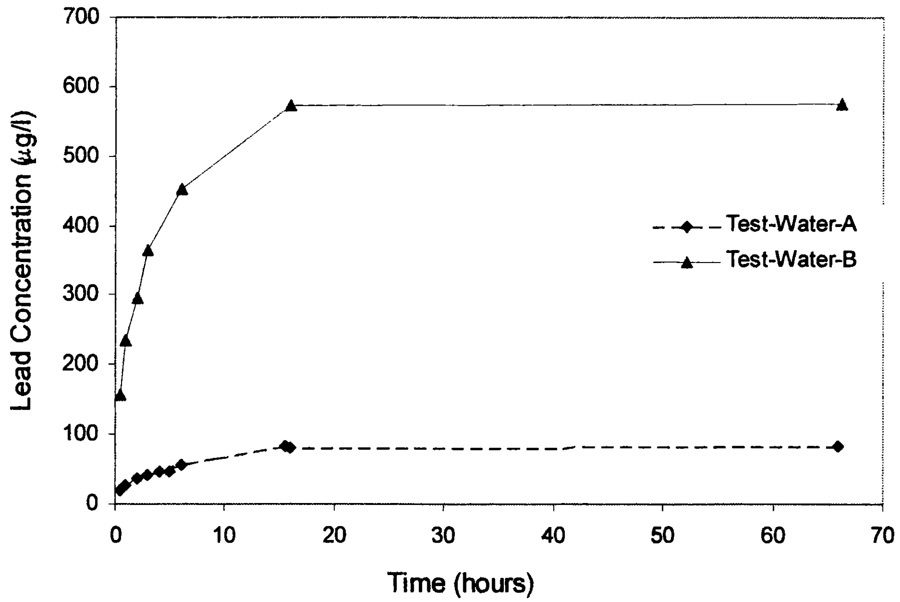


Figure 2.53. Stagnation curves for two contrasting test waters.

Note that the data points for Test-Water-B are average values of the three lead pipes, while those for Test-Water-A are average values of pipe-2 and pipe-3 only, since the results from pipe-1 were particularly erratic and considered to be erroneous.

As predicted by the diffusion model, the experimental data points for both test waters form a characteristic stagnation curve, where the mass transfer rate reduces with stagnation time until an equilibrium concentration is reached. However, the equilibrium concentrations for both test waters are somewhat higher than expected. This was later found to be due to the effect of temperature on lead dissolution. The typical equilibrium concentrations, previously outlined (Chapter 1.2.3.2) assume that the lead pipe is underground at a temperature of around *5-10°C*. This contrasts to a typical ambient temperature of around *20°C* recorded during the experiments. With reference to Figure 1.6, it can been estimated that this increase in temperature has the effect of increasing the equilibrium concentration by a factor of approximately two.

In addition to the established relationship between concentration and stagnation time, several other parameters have shown some form of relationship, in particular pH and stagnation time (Figure 2.54). This relationship has been found to be of similar shape to the stagnation curve itself as illustrated by the inclusion of a 'transformed' diffusion function fitted to the experimental data. This phenomenon is probably caused by the transfer of calcium carbonate or similar pH elevating substances from the corrosion deposit into the stagnating water. Since the physical mechanism governing mass transfer during stagnation is diffusion, it follows that the increase in pH will also follow a diffusion function.

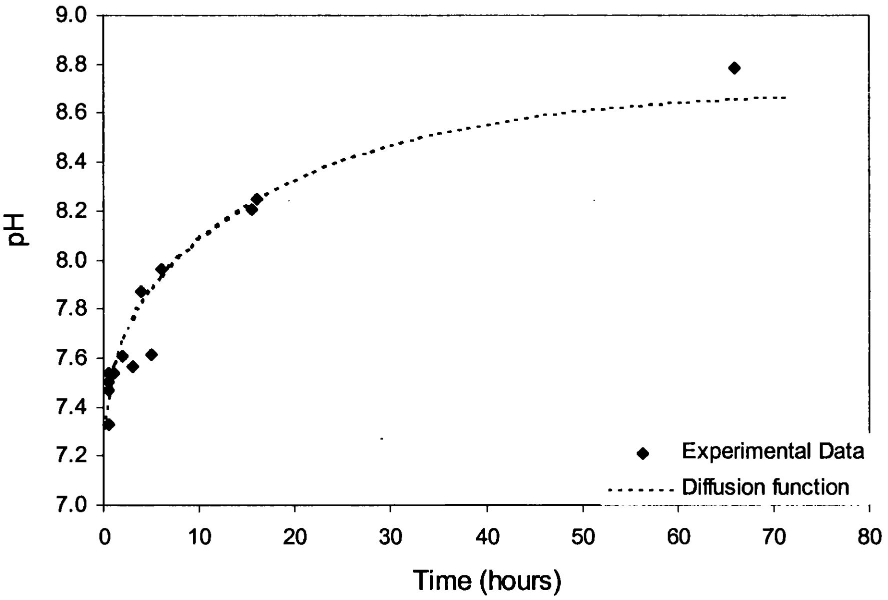


Figure 2.54. Relationship between sample pH and stagnation time.

2.5.4 Calibration of the diffusion model

The diffusion coefficient, *D* and the equilibrium or solubility concentration, *E* must be obtained in order to calibrate the diffusion model. By setting *E* to the maximum concentration in Figure 2.53, a suitable value of *D* can be obtained by calibration of (Eqn. 2.46) with experimental data for each test water. Calibration is carried out using least-squares curve fitting of the diffusion model to the experimental data. This has also allowed the overall closeness of fit of the experimental data and the diffusion model to be assessed visually (Figure 2.55).

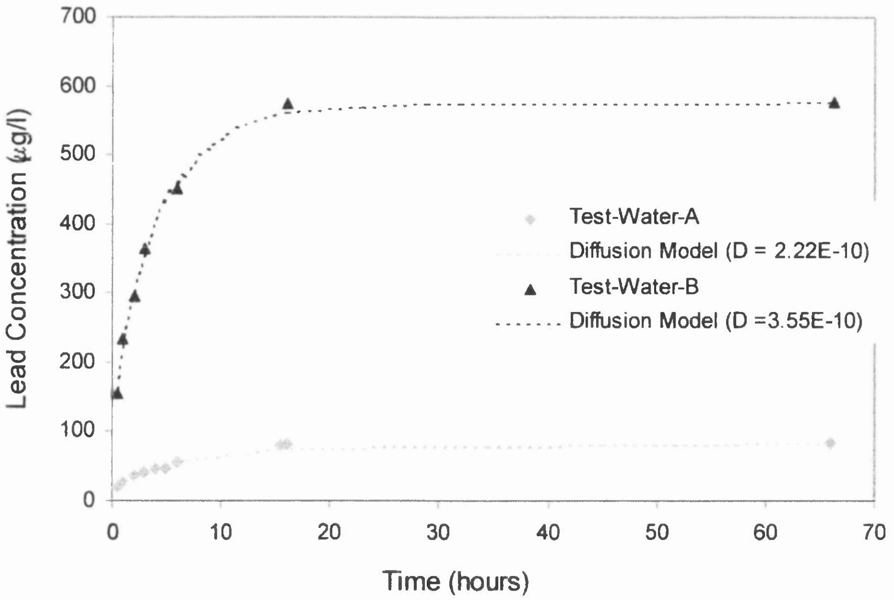


Figure 2.55. Calibration of diffusion model to experimental data.

From this plot it is clear that the experimental results can be fit very closely to the predicted diffusion model values. A diffusion coefficient of $D = 3.55E\text{-}10\ m^2/s$ has been obtained for Test-Water-B. This compares favourably when calibrating to the *30MS* value of the exponential model where the diffusion coefficient was found to be $D = 4.46E\text{-}10\ m^2/s$ (Chapter 2.3.1). This is also in general agreement with the diffusion coefficient of $D = 5.00E\text{-}10\ m^2/s$ used by Cardew [53] despite being associated with a different water. Kuch and Wagner [50] quote a diffusion coefficient of $D = 10.00E\text{-}10\ m^2/s$ used in their calculations of lead concentration. This is significantly higher than the values predicted, possibly because the water used in experiments by Kuch and Wagner was significantly more acidic.

However, the diffusion coefficient obtained for Test-Water-A is significantly lower at $D = 2.22E\text{-}10\ m^2/s$, as is the equilibrium concentration. This is because the equilibrium concentration is achieved at approximately the same time for both test waters, despite differences in equilibrium concentration.

3 WATER SUPPLY ZONES

3.1 Mathematical description of a water supply zone

3.1.1 Introduction

Through the application of the mathematics of mass transfer and fluid flow, lead emissions at a single property have been modelled in great detail. This has facilitated the study of the influence of parameters, such as pipework and water usage, on lead emissions, both as a daily average value and at various times throughout the day. However, in order to understand the general issues that relate to plumbosolvency control on a zonal scale, it is necessary to model the structure of an entire water supply zone. This will enable the prediction of zonal compliance with the lead standards as well as the investigation of the likely effects of corrective water treatment and selective lead pipe replacement in order to facilitate the optimisation of plumbosolvency control measures.

The average water supply zone in the U.K. has a population of slightly more than 20,000 people, which translates to 10,000 houses, of which approximately 40% are supplied through lead pipework. However, influencing factors such as pipework configuration and water usage often vary considerably across a single water supply zone, which results in a wide range of lead emissions being observed. Consequently, in order to accurately predict zonal compliance, it is essential to model the extent and shape of the wide variation that occurs across real water supply zones. Additionally, the zonal model to be developed must be highly flexible to facilitate best possible calibration to real-world zones.

3.1.2 Structure of a zone

It is not logistically practical to develop a completely accurate description of a real-world water supply zone in terms of pipework configurations, consumer behaviour and water quality variation. However, a general description of a water supply zone can be developed by defining the method in which the relevant data for a water supply zone is structured. Such relevant data includes the general properties of the water supply zone, such as size, as well as properties that vary throughout the zone, such as length of pipework. This 'framework' of a zone can be used to develop an accurate model of a real zone through calibration with data obtained through surveys and investigations.

In the simplest case, where there are no shared communication pipes, a zone consists of a set of independent houses connected to the water main. The houses can be assumed to be independent in every sense, i.e. the properties that influence lead emissions at a particular house, as well as the actual lead emissions observed at that house, do not effect the properties or emissions at any of the remaining houses in the zone.

Consequently, the data required to describe a zone can essentially be structured into a list of houses and the household properties at each house. This zonal data can be stored in an array as:

$$Zone[Address(i), Household\_Properties(i)] \quad \text{for } i = 1, H_T \qquad \text{Eqn. 3.1}$$

where H_T is the total number of houses in the zone. Note that *Address* is simply a reference number for a house.

3.1.3 Fixed quantities

The elements that define a water supply zone fall into two main categories, namely fixed quantities and variable quantities. Fixed quantities define:

- General properties of the zone as a whole.
- Parameters that effect lead emissions but remain constant across the water supply zone.

General properties of a zone include the total number of houses, H_T, and the proportion of houses supplied through lead pipework, *Pb%*.

In order to ensure maximum flexibility of the zonal model, it is necessary to assume that all household parameters can be applied as varying quantities when necessary. However, if the effect on lead emission of a parameter is negligible, or the variation of this parameter across the zone is insignificant, then the parameter should be applied as a constant. Examples where parameters should be applied as constants include:

- Pipework diameter. Although pipework diameter has a significant effect on lead emissions, its variation across water supply zones in the U.K. is generally negligible, with the vast majority of plumbing being of 12mm internal diameter.

- Flow rate. Flow rate is usually in the order of *0.1l/sec* for typical residential use, though will vary to some degree. However, the effect of flow rate on lead emissions is small (Chapter 2.4.2.7).

- Plumbosolvency. For most water supply zones, particularly where the water being supplied is of high alkalinity, the quality of water throughout the zone is fairly uniform; consequently the plumbosolvency of the water does not vary appreciably.

3.1.4 Variable quantities

Variable quantities define the household parameters that:

(a) Have an effect, no matter how small, on lead emissions at that house.

as well as satisfy one or more of the following statements:

(b) Parameter has a marked influence on lead emissions.
(c) Parameter has a large variation across the zone.

Through investigations of the influence of factors, such as pipework and water usage, on lead emissions, previously described (Chapter 2.4.2), it has been found that the following household parameters satisfy condition *(a)* above:

- Length of Lead Pipework
- Length of Copper Pipework
- Diameter of Pipework
- Flow Rate (when the tap is on)
- Total Volume of Water Used (in one day)
- Pattern of Water Usage

- Plumbosolvency parameters (*M* and *E* or *D* and *E*)

In the case of some real-world zones, it is clear that some of these parameters could be considered zonally static since they will not satisfy either condition *(b)* or *(c)*. However, for flexibility, it is assumed that all of the above parameters could, in theory, also satisfy *(b)* or *(c)* and thus must be able to be applied as variable quantities. Consequently, values of each of these parameters must be stored for every house in the zone and (Eqn. 3.1) becomes:

$$Zone[i,j]$$

$$for\ i = 1,\ H_T;\ j = 1,\ 8$$

$$where$$

$$\begin{aligned} j(1) &= Address(i) \\ j(2) &= L_{Pb}(i) \\ j(3) &= L_{Cu}(i) \\ j(4) &= PD(i) \\ j(5) &= Q(i) \\ j(6) &= V^T(i) \\ j(7) &= WP(i) \\ j(8) &= Plumb(i) \end{aligned} \qquad \text{Eqn. 3.2}$$

Where L_{Pb}, L_{Cu}, *PD*, *Q*, V^T, *WP and Plumb* are length of lead pipework, length of copper pipework, diameter of pipework, flow rate, total daily water consumption, pattern of water usage and plumbosolvency respectively.

3.1.4.1 Statistical representation

It is clearly not logistically practical to quantify household parameters for every single house in a real-world water supply zone. Consequently, it is necessary to be able to model a real-world zone using the limited data obtained through surveys and investigations. Qualitative data from real-world zones can be used to define the general characteristics of how each parameter typically varies throughout a zone. It is sometimes found that a standard statistical distribution, such as the Normal distribution, is adequate for representing the real-world variation of a household parameter. The exact shape of each distribution can be modified in order to represent the extent of variation required.

The general shape of the Normal distribution tends to be closely approximated by the distributions of a very large number of real-world empirical variables [75]. The Normal distribution is a theoretical distribution generated by a formula known as the normal probability density function (Eqn. 3.3), which describes how probability density varies with the value of the parameter *y*. This function is continuous in nature, meaning that the value of the parameter can take on any real-number value within a certain range.

$$f(y)=\frac{\exp\left[-(y-\mu)^2/2\sigma^2\right]}{\sigma/2\pi} \quad \sigma \geq 0, -\infty \leq \mu \leq \infty, -\infty \leq y \leq \infty \qquad \text{Eqn. 3.3}$$

The parameters that define the Normal distribution are the mean μ, which defines the effective 'middle' of the distribution, and the standard deviation σ, which defines the variability or 'spread' of the distribution.

Probability is represented as the area under the standard normal distribution curve; the area under the entire curve representing 100% probability. The curve extends to infinity in both directions, however the probability of obtaining an extreme value is very small, though still theoretically possible. Consequently, it is necessary to impose cut-off points at the extremes in order to ensure that there is zero probability of obtaining an unrealistically low (or negative) value or an unrealistically high value (Figure 3.1).

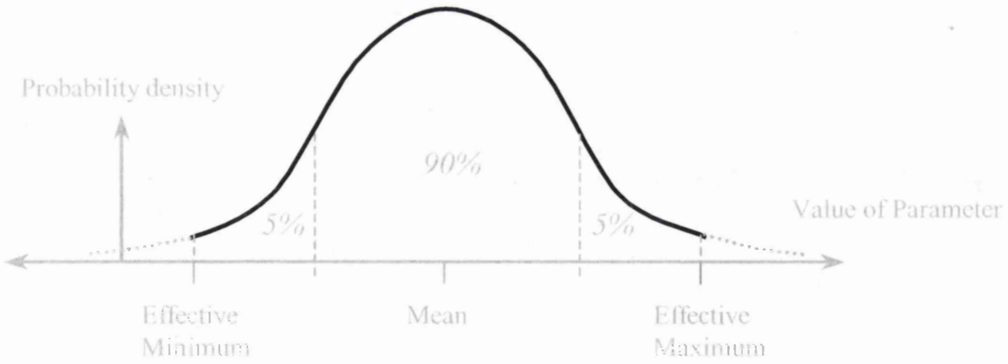


Figure 3.1. Normal distribution.

Survey data from real zones suggests that some household parameters appear to form a Log-Normal distribution, i.e. the logarithm of the parameter follows a normal distribution [61]. This results in an asymmetric distribution, skewed towards smaller values of the parameter (Figure 3.2).

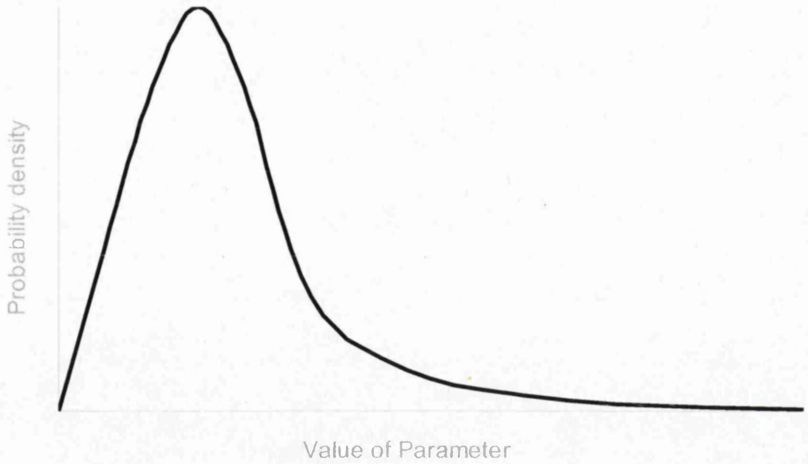


Figure 3.2. Log-Normal distribution.

General distributions, such as the Normal and Log-Normal distribution, in some cases, can be calibrated closely to real-world zonal data in order to represent the extent and shape of variation of zonal parameters.

3.2 Modelling a water supply zone

3.2.1 Distribution of house variables

For an arbitrary water supply zone, where there is no available survey data relating to household parameters, details of the distribution of the parameters must be assumed. In this case, assumptions are based on general knowledge of water supply zones [61], qualitative data from real-world zones, and common sense. For a specific real-world water supply zone, appropriate survey data, where available, can be employed together with any necessary assumptions in order to calibrate the zonal model as far as possible.

In order to facilitate the input of zonal data, particularly where it is available directly from survey data, distributions of household parameters will be represented in discrete form rather than continuous form. This will result in a list of discrete values and corresponding probability (or percentage of total), for each household parameter. The motivation for employing discrete distributions is to facilitate flexibility of the model and overcome limitations associated with representing data using theoretical distributions. The primary limitation of theoretical distributions is that they cannot always mimic the shape or extent of survey data from real-world zones. This is because:

- Artificial cut-off points must be imposed on the theoretical distribution, as previously described.
- Ambiguity of input parameters for the theoretical distribution.
- Kurtosis (whether the shape of a distribution is relatively short and flat, or tall and slender) and level of Skew of survey data is complicated to represent using theoretical distributions.
- More complex distributions, such as those having more than one mode (peak) must be modelled using a combination of theoretical distributions, which further compounds the problem of calibration.

Additionally, survey data from real-world zones is exclusively discrete, thus its input into a model employing discrete distributions is straightforward. Furthermore, there is little point accurately defining a theoretical distribution when real-world data is limited with only a basic outline of a distribution available. When limited data is available, the discrete distribution can be very course, i.e. the increments in parameter values are large. However, if an extensive survey of a real-world zone has revealed more detailed data, such as the number of houses having lead pipework of *1m, 2m, 3m, 4m...etc*, then this can be represented exactly, simply by using a *1m*-fine discrete distribution.

When there is very limited survey data, the distributions of household parameters are assumed to have standard characteristics that have frequently undergone peer review without significant change. These characteristics will be described and justified for each household parameter.

3.2.1.1 Pipework

Length of lead pipework has been found to significantly effect household lead emissions (Chapter 2.4.2.2) and has also been found to vary significantly across water supply zones. Surveys have revealed that in some isolated situations, the lead pipework used to supply a property can be as long as *70 – 100m*; though in most cases it has been found to be fairly short, of the order of *5 – 20m*. Consequently, it is logical to assume that zonal variation of lead pipework follows an asymmetric distribution, biased towards shorter lengths. This skewed distribution is characteristic of a Log-Normal distribution, having a mean of approximately *15m*, after which the proportion of houses having longer lead pipework rapidly decreases (Figure 3.3). Note that this histogram does not include households that do not have lead pipework.

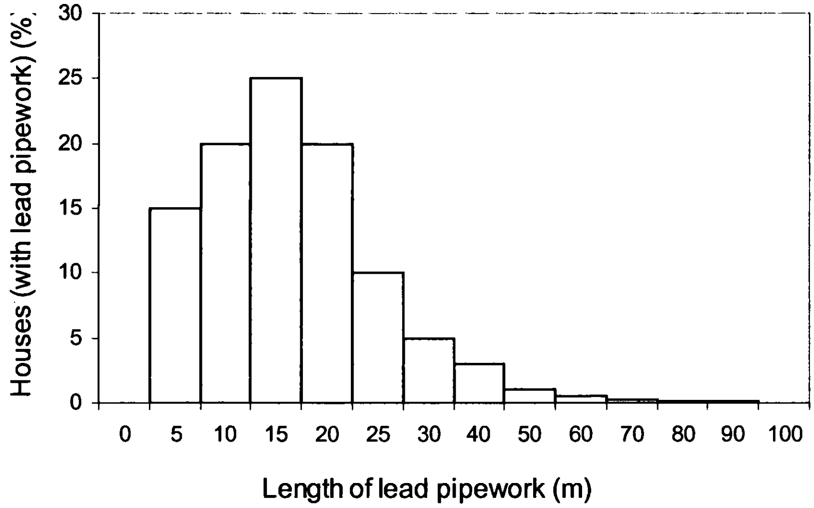


Figure 3.3. Distribution of lead pipework length.

Non-lead (copper) pipework is often present at properties that have a lead communication pipe because the internal lead plumbing is often replaced using a non-lead material, usually copper. Although the length of copper pipework has no effect on lead emissions in terms of daily average concentration (*DAC*), it does have a significant effect on *30MS*. It is also likely that the length of copper pipework will vary significantly across a water supply zone due to the diversity of plumbing installations.

It is possible that households with lead pipework could have very long copper pipework, though in most cases the length of copper pipework will be smaller than the length of lead pipework, where present. This is because lead pipework is usually present in the form of the longer communication pipe or service pipe, which typically runs several feet underground from the road to the house, while copper pipework is usually present in the form of the shorter internal plumbing. Consequently, it is logical to assume that zonal variation of copper pipework follows an asymmetric distribution, biased towards shorter lengths, as is the case of lead pipework. However, for properties with lead pipework, the mean length of copper pipework is likely to be shorter than that for the lead, as reflected by the assumed distribution (Figure 3.4).

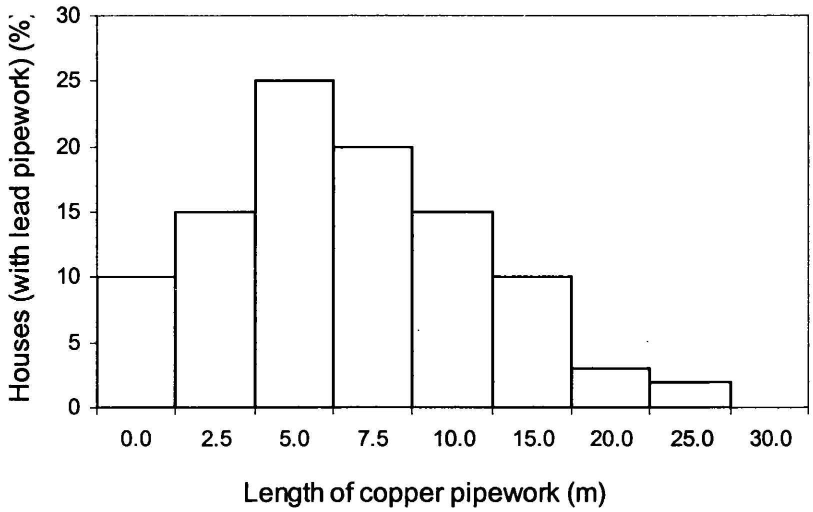


Figure 3.4. Distribution of copper pipework length.

In the UK, the internal diameter of pipework between the water mains and the tap is generally found to be *12mm*. Thus, pipework diameter is ordinarily applied as a constant value of *12mm* across a water supply zone. However, pipework diameter can be specified as a weighted range when survey data reveals a variation in this parameter.

3.2.1.2 Plumbosolvency

Plumbosolvency, as defined by the parameters M and E or D and E, is ordinarily applied as a constant value across a water supply zone. These parameters are calibrated by reference to "over-night standing" and "30-minute stagnation" samples taken from properties within the zone. However, if there is evidence to suggest that the zone suffers from distinct changes in water quality, where pH reduces as the water passes through the distribution system, then plumbosolvency can be specified as a weighted range (Figure 3.5).

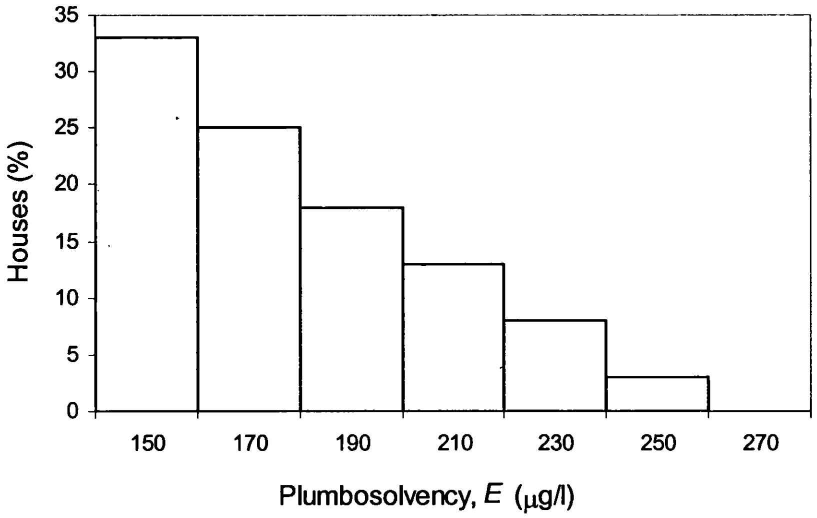


Figure 3.5. Distribution of plumbosolvency.

Figure 3.5 illustrates a typical variation that may occur for a low alkalinity moderately plumbosolvent water, which has a poor buffering capacity, i.e. suffers a pH reduction as the water passes through the distribution system. Although the solubility of drinking water leaving the water works is *150μg/l*, it can increase significantly at the extremities of the water supply zone, where the pH reduction, and therefore corrosivity of the water, is highest.

3.2.1.3 Water usage

Flow rate is usually in the order of *0.1l/sec* for typical residential use, though will vary to some degree. However, the effect of flow rate on lead emissions is small (Chapter 2.4.2.7). Thus, flow rate is applied as a constant value of *0.1l/sec* across a water supply zone.

Conversely, daily water consumption has been found to significantly effect household lead emissions (Chapter 2.4.2.5) and has also been found to vary significantly across water supply zones, increasing with the number of occupants [62]. In the absence of relevant survey data, it is logical to assume that the zonal variation in daily water consumption follows a Normal distribution (Figure 3.6), since the number of occupants per household will approximately follow a Normal distribution. Previous experience [61] suggests that the average household will use between *300l* and *600l* of water each day. Consequently, the mean of the applied distribution is *450l*, with increments to a minimum value of *50l*, representative of a conscientious single occupant, and a maximum value of *850l*, representative of a large imprudent family.

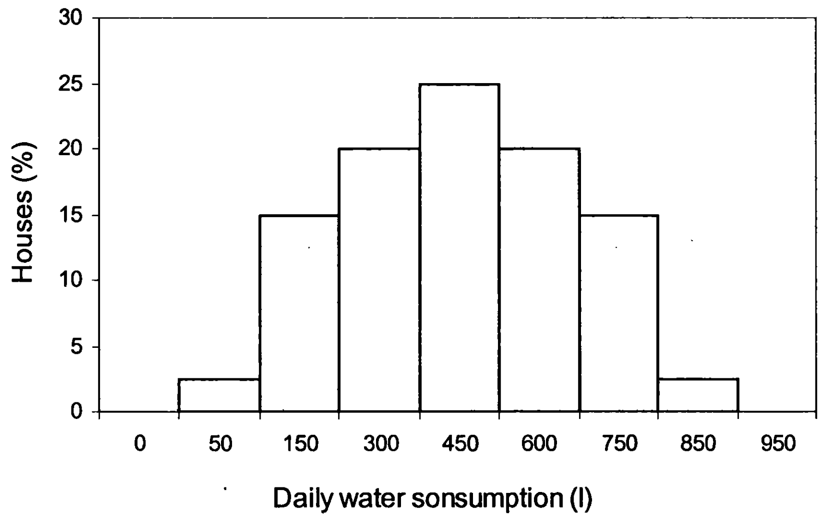


Figure 3.6. Distribution of daily water consumption.

A range of different water usage patterns must be applied to the zone in order to model the zonal variation in consumer behaviour with respect to the pattern of water usage. Data regarding water usage patterns in real-world zones is very limited, thus it is necessary to apply a number of assumed patterns, each characterised by a general shape as well as a flow frequency. There are two basic shapes of water usage pattern, these being derived through previous experience and studies [62]:

- Type-A: describes a house with residents at home throughout the day (Figure 3.7).
- Type-B: describes a house in which there are no residents at home during the working day (Figure 3.8).

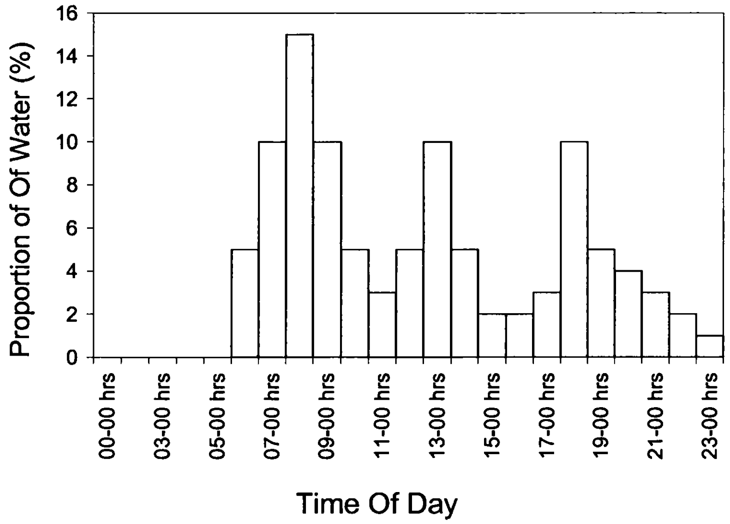


Figure 3.7. Water pattern (Type-A).

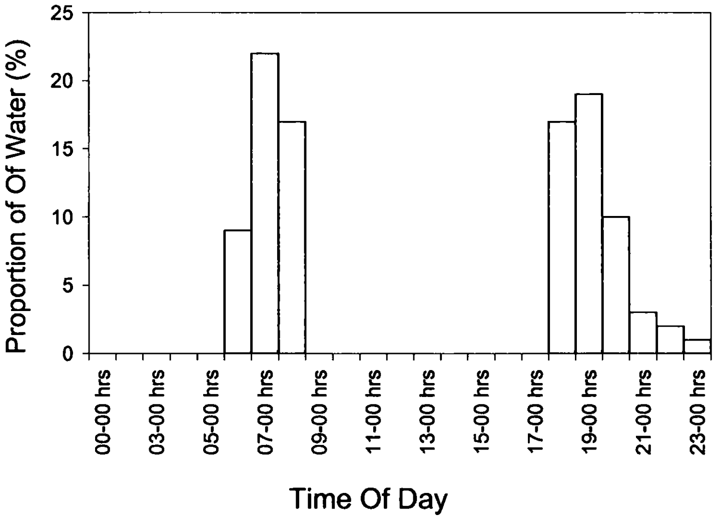


Figure 3.8. Water pattern (Type-B).

In addition to the basic shape of the water usage pattern, it is necessary to apply a range of flow frequencies across the zone. This is because the flow frequency, as defined by the mean inter-use time, has been found to be dependent on household size and the number of occupants [62]. Obviously, flow frequency will increase with increasing number of occupants. Accordingly, type-A is applied using (a) half-hourly, (b) quarter-hourly and (c) eighth-hourly flow event frequencies, whilst only (b) and (c) are used for Type-B. The aim is simply to impose an appropriate proportion and range in water use patterns to mimic zonal circumstances over a period of at least one year. These five different water usage patterns are applied evenly across the water supply zone.

3.2.2 Monte Carlo simulation

It is possible to characterise the zonal variation of household parameters using discrete distributions, as previously described. However, in order to describe the properties of each house in the zone, it is necessary to ascribe values to each house from each distribution of household parameters. Since a typical zone comprises *10,000* houses, it is clearly not practical to manually ascribe these values to every single house in a zone, thus ascription must be fully automatic.

In order to mimic the extent and shape of the wide variation in household parameters that occurs across real water supply zones, the ascription of parameters must be independent of the house. This will potentially permit any combination of values of household parameters to occur at each house, e.g.:

- Large lead pipework + Large water consumption
- Large lead pipework + Small water consumption

- Small lead pipework + Large water consumption
- Small lead pipework + Small water consumption

A standard numerical technique known as the Monte Carlo method can be employed for the purposes of simulating the zonal lead emissions that occur. A Monte Carlo method is defined as any technique that involves the use of statistical sampling procedures to approximate the solution of a mathematical or physical system [76], in this case lead emissions across a water supply zone. 'Monte Carlo methods have been used for centuries, but only in the past several decades has the technique gained the status of a full-fledged numerical method capable of addressing the most complex applications. Monte Carlo is now used routinely in many diverse fields, from the simulation of complex physical phenomena such as radiation transport in the earth's atmosphere and the simulation of the esoteric sub-nuclear processes in high energy physics experiments, to the mundane, such as the simulation of a Bingo game' [77]. The method has also been used extensively in the field of environmental modelling, in particular determining water quality of rivers [78,79].

The Monte Carlo method involves randomly ascribing a value from each distribution and then evaluating the solution, in this case lead emissions, at that house. Repeated sampling simulates the many combinations of household parameters that occur in real water supply zones. The results form a statistical description of the systems behaviour, i.e. the distribution of household lead emissions that occur across the zone. A larger number of samples result in a more accurate description of the system's behaviour since more combinations of household parameters can be simulated and sampling error reduces.

The random selection of a value, *X* from a distribution of a household parameter is carried out as follows:

- Generate a random number, *Rand* (between 0.0000 and 1.0000). This can be accomplished through use of random number tables or computerised random number generators.
- Set *Rand* to the probability of obtaining a value of *X* or less (i.e. the area underneath the distribution to the left of *X*.
- Calculate *X* (from discrete data describing the distribution of the household parameter)

To illustrate this process, an example of randomly ascribing a length of lead pipework of *10m* to a house, from a random number of *0.2500*, is illustrated (Figure 3.9).

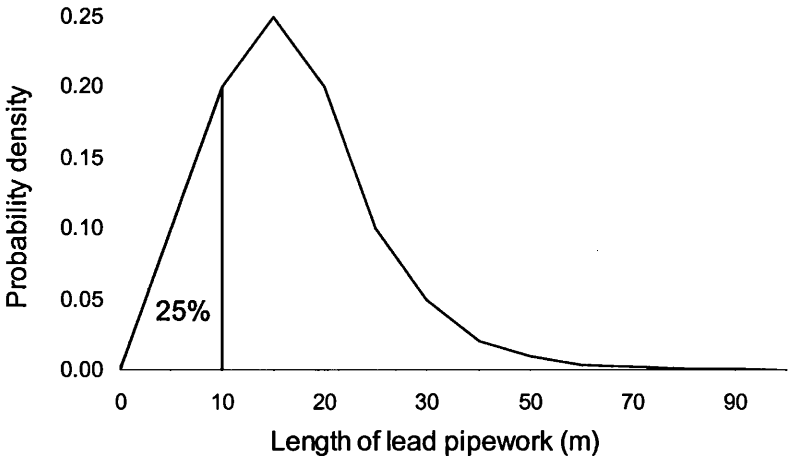


Figure 3.9. Random selection of lead pipework length (*Rand* = *0.25*).

3.2.3 Generation of zone

It is clear that the capability to model the daily average concentration of lead for a single house, previously described, can be extended to an entire water supply zone through the application of the Monte Carlo method. This will result in a prediction of the zonal compliance with the lead standards that is completely representative of the weekly average value ingested by consumers (a primary aim of this research).

In order to maintain flexibility, a complete description of the zone, with respect to the household properties at every single house, must be stored for potential subsequent investigation. Consequently, the Monte Carlo method will be employed in a modified process, where the random ascription of household parameters for the entire zone is carried out prior to the evaluation of lead emissions, as follows:

- For every house in the zone
    - Randomly ascribe values from each distribution of household parameters
    - Store parameters for house
- Evaluate lead emissions across the stored zone in accordance with the method of compliance assessment (covered in the following subchapter).

The process of generating and storing a complete description of a zone is illustrated (Figure 3.10).

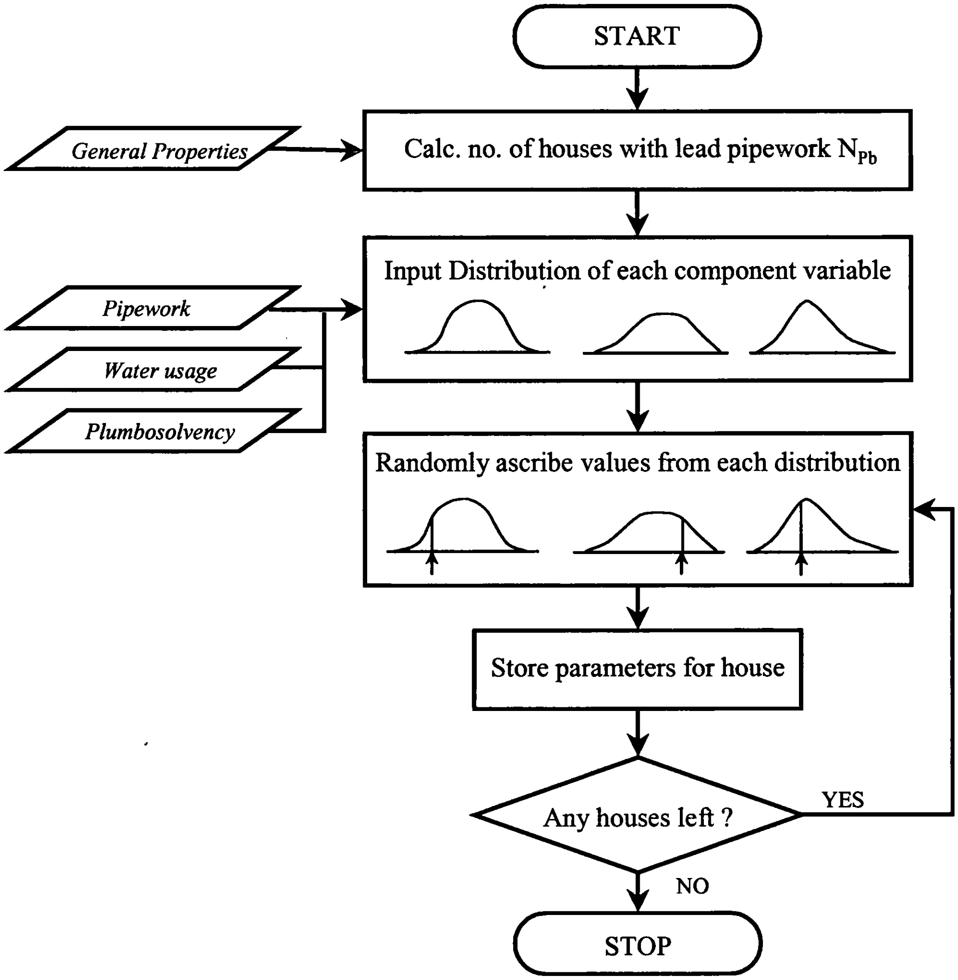


Figure 3.10. Generating a zone.

3.2.4 Simulation of compliance assessment

The configuration of a real-world water supply zone can be modelled using the Monte Carlo method by generating and storing a complete description of the zone, with respect to the household properties at every single house. However, in order to predict zonal compliance with the lead standards or investigate the likely effects of corrective water treatment, it is necessary to evaluate lead emissions across the stored zone in accordance with the method of compliance assessment. There are several methods of assessing compliance that can be simulated; these include 'exact' assessment, which can only be performed with a computational model, as well as a number of real-world sampling protocols.

'Exact' assessment is the most comprehensive method of determining zonal compliance in accordance with the new directive and involves the characterisation of all lead emissions occurring across a zone. The capability to simulate various real-world sampling protocols is necessary to characterise the behaviour of a simulated zone in a way that can be validated to real sampling data collected by water companies. This will also enable different sampling protocols, which are currently employed by water companies, to be evaluated in terms of suitability for demonstrating the optimisation of corrective water treatment.

3.2.4.1 Exact assessment of compliance

The 'exact' assessment is the most accurate method of measuring compliance with the lead standard in accordance with the new EU "drinking water" directive. As described previously, the new "drinking water" directive indicates that the parametric values of $10\mu g/l$ and $25\mu g/l$ apply to a sample of water intended for human consumption (that is from the consumer's tap) obtained by an adequate sampling method and taken so as to be representative of a weekly average value ingested by consumers [32].

Through the use of computational modelling, some real-world limitations can be overcome and an exact assessment of zonal compliance can be estimated by computing the *DAC* for every single house in the zone. Computing *DAC* results in a completely representative value for the daily average concentration of lead ingested by consumers from drinking water. The closest real-world equivalent of computing *DAC* is the concentration obtained from composite proportional (*COMP*) sampling of a property, described previously. By virtue of taking into account the daily variations in lead emissions, *DAC* eliminates the poor reproducibility associated with traditional *RDT* sampling that is caused by the wide variation in lead emissions that can be expected at a single property over the course of the day. It should be noted that the *DAC* is an adequate surrogate for weekly average concentrations because of the way in which the water use patterns are applied in the zonal description.

Additionally, instead of sampling a necessarily limited number of houses within the zone, computational modelling can enable lead emissions to be evaluated at every single house in the zone. This overcomes the poor reproducibility associated with traditional *RDT* sampling that is caused by the wide variation in lead emissions that occur throughout the zone.

Note that by taking into account all variations in lead emissions, both throughout an entire day and throughout the entire zone, the exact assessment effectively eliminates the uncertainty inherent in traditional sampling. The resulting zonal compliance obtained with this method will remain constant for a fixed water supply zone, i.e. the method is completely reproducible. Thus, any change in zonal compliance must be a result of changes to the parameters describing the zone, such as plumbosolvency, and not a result of chance.

An exact assessment of zonal compliance is simulated by applying the model for a single house to each address within the stored description of the zone that has lead pipework, since there are no lead emissions at houses having no lead pipework. The *DAC* computed for each house is then compared to a number of lead standards, such as *10µg/l*, *25µg/l*, and *50µg/l*, and zonal failure rates, i.e. the percentage of houses in the zone where the *DAC* exceeds these standards, are computed. This exact assessment simulation can be characterised by the flow diagram illustrated (Figure 3.11).

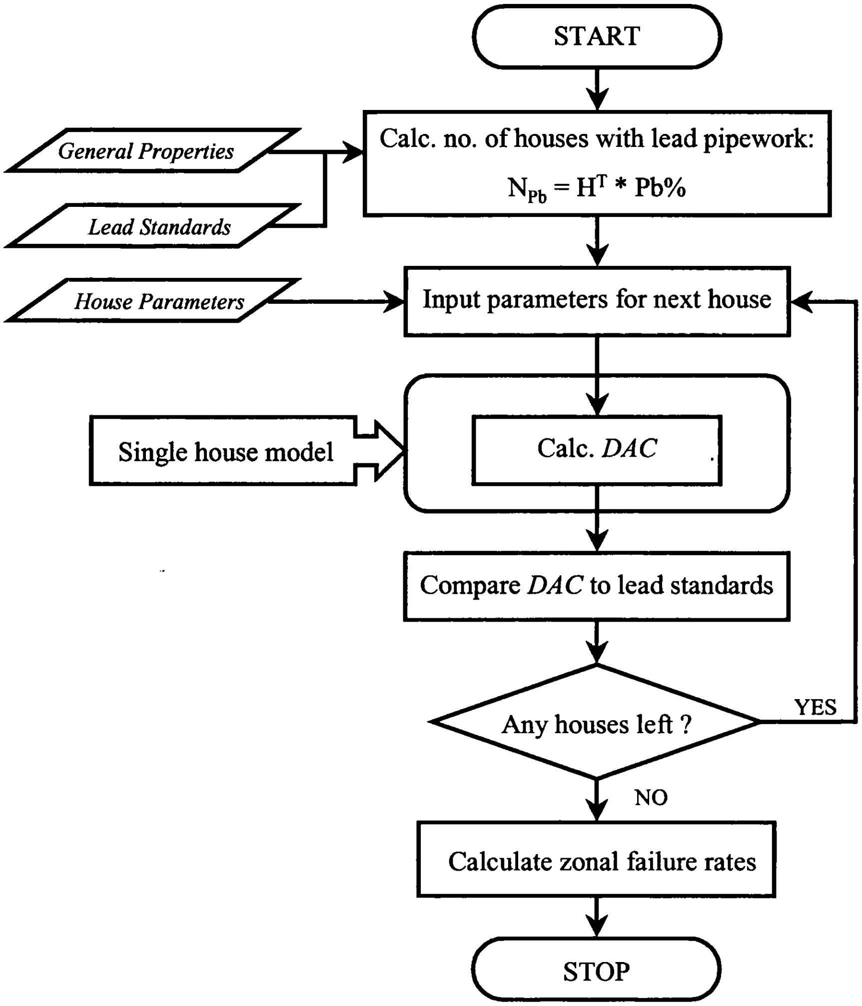


Figure 3.11. Simulation of exact zonal compliance assessment.

It should be noted that each house is modelled as being independently connected to the water mains, i.e. there are no shared communication pipes; thus lead emissions at a house are not influenced by other houses in the zone. This is a reasonable assumption considering that most water supply zones in the U.K. consist of housing that is almost exclusively detached, semi-detached or terraced. In these cases the properties are supplied with drinking water from the water main via a single communication pipe as depicted in Figure 1.5.

Clearly it is possible to compute *DAC*, and therefore zonal failure rates, using any of the available combinations of mass transfer and flow models to model lead emissions at a single house, as previously illustrated (Figure 2.13).

3.2.4.2 RDT sampling

The capability to simulate various sampling protocols is necessary in order to characterise the behaviour of a simulated zone in a way that can be validated to the real-world data collected by the water company. This is because there is no real-world data relating to exact methods of assessing zonal compliance since, in reality, this method would entail the installation of composite proportional (*COMP*) sampling devices in every single house in the zone; this is clearly not logistically possible.

The simulation of sampling protocols that are currently employed by water companies will enable each protocol to be assessed in terms of:

- how accurately they predict the exact compliance with the new lead standards.
- how suitable they are for use in the optimisation of corrective treatment.

Of particular importance is the ability to simulate *RDT* sampling, since this is currently the most widely employed method of assessing compliance in the UK. As a consequence of simulating *RDT* sampling, it will be possible to investigate the reproducibility and possible variation in results by repeatedly simulating *RDT* sampling surveys. *RDT* sampling at a single house involves the taking of a one-litre sample directly from the kitchen cold-water tap of a randomly selected property at a random time during the working day (i.e. between 9am and 5pm), without flushing any water beforehand. It should be noted that in the UK, water companies have been required [25] by the regulations to assess compliance with the lead standard in this manner.

This process is simulated by randomly selecting a sampling time during the simulated day, i.e. between 9am and 5pm, to take the sample. This is achieved through the following process:

- Generate a random number, *Rand* (between 0.0000 and 1.0000). This can be accomplished through use of random number tables or computerised random number generators.
- Calculate the length of time from 9am to the sampling time as *LT(hours) = Rand * (8 hours)*

- Calculate sampling time as $ST = 9 + LT$

The simulation of every single flow and stagnation event during the simulated day of water usage is then run as described in Chapter 2.2.5, up to the pre-selected sampling time *LT*, at which point the sample is to be collected. The sample collection itself is then simulated by calculating the average concentration of lead during a flow period of sufficient length to allow one litre of water to be drawn from the tap. It should be noted that this method of simulating *RDT* sampling fully takes into account the water usage throughout the day up to the point of taking the random daytime sample.

As with exact assessment, it is possible to compute *RDT* sample concentrations, and therefore zonal failure rates, using any of the available combinations of mass transfer and flow models to model lead emissions at a single house, as previously illustrated (Figure 2.13).

In order to simulate a complete *RDT* sampling survey, which typically comprises *50 – 100* samples, a specified number of houses are selected at random from the zone. This is readily achieved through the use of a random number generator. However, it should be noted that in practice if access to the selected property is not possible, i.e. there are no occupants at home, then the house next door is tried, and so on, until access is gained. Consequently, it is necessary to examine the water usage pattern of the selected house to see if occupants are home between *9am* and *5pm*, i.e. if any water is used between *9am* and *5pm*. If water is not used during this period then it must be assumed that there are no occupants are present during the working day, and hence the next house must be tried.

The *RDT* sample concentration computed for each house is then compared to a number of lead standards, such as *10μg/l*, *25μg/l*, and *50μg/l*, and zonal failure rates, i.e. the percentage of houses in the zone where the *RDT* sample concentration exceeds these standards, are computed. However, since *RDT* sampling survey results are never completely reproducible, it is necessary to repeat the simulated survey, typically *100* times, in order to be able to understand possible variation. The *RDT* sampling simulation can be characterised by the flow diagram illustrated (Figure 3.12).

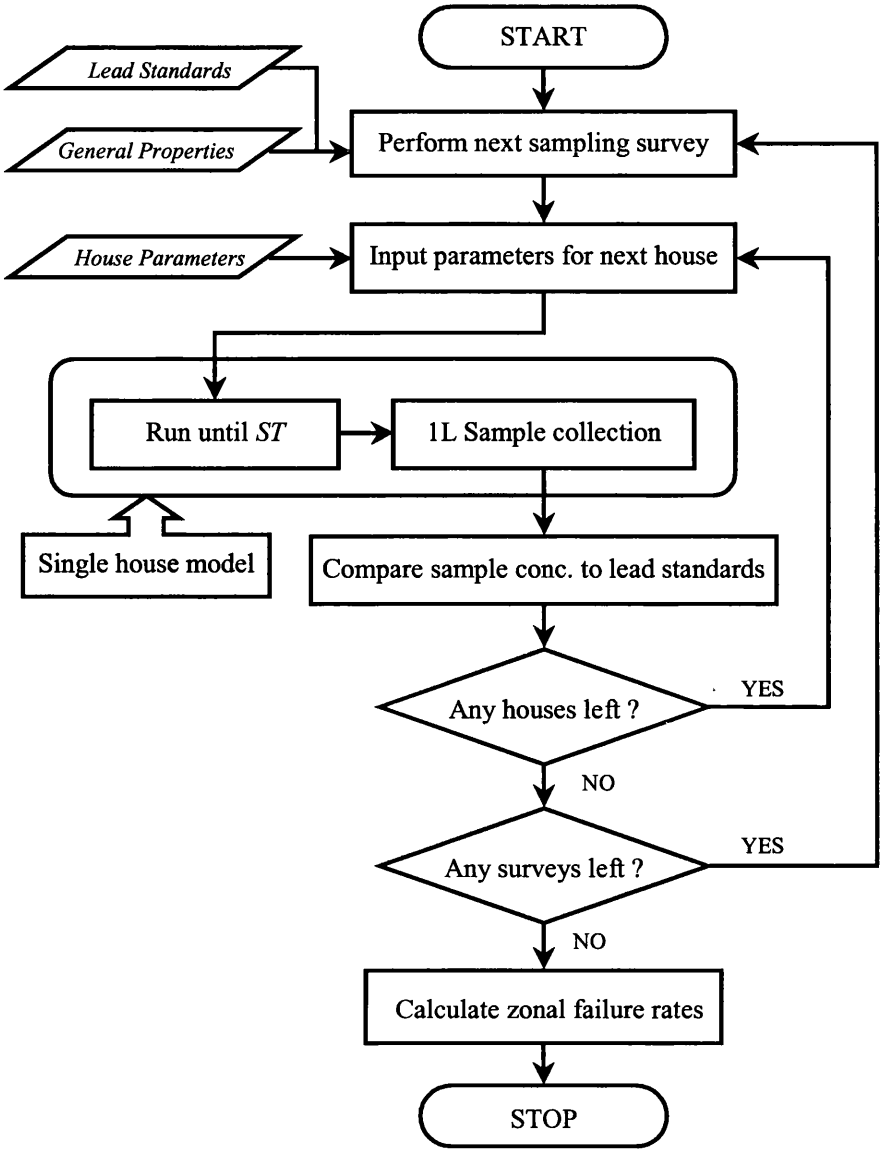


Figure 3.12. Simulation of multiple RDT sampling surveys.

In order to facilitate the investigation of the possible variation in results obtained through simulation of multiple sampling surveys, various statistics must be calculated. Of particular importance are the mean $\overline{F}$ and standard deviation σ of the number of samples in a survey that fail F for each water quality standard. For m simulated sampling surveys, these statistical parameters are computed as:

$$Mean = \overline{F} = \frac{1}{m}\sum_{i=1}^{m} F_i \qquad \text{Eqn. 3.4}$$

$$StandardDeviation = \sigma = \sqrt{\frac{m\sum_{i=1}^{m}\overline{S}_{Fail,i}^{\,2} - \left(\sum_{i=1}^{m}\overline{S}_{Fail,i}\right)^2}{m^2}} \qquad \text{Eqn. 3.5}$$

3.2.4.3 Other sampling methods

Although *RDT* sampling is currently the most widely employed method of assessing compliance in the UK, a number of other sampling methods exist. These include *COMP* sampling, which is arguably the most accurate method of characterising lead emissions at a single house, and *6-hour* stagnation sampling, which is widely used in the USA in accordance with the US-EPA "lead and copper rule" [31].

As with *RDT* sampling, these methods involve the random selection of a specified number of houses from the zone; this is readily simulated using a random number generator. Consequently, such sampling survey results will never be completely reproducible, and it is necessary to repeat the simulated survey, typically *100* times, in order to be able to understand possible variation. Thus, the general framework of simulating *RDT* sampling surveys, as characterised by Figure 3.12, can be employed for other sampling methods. Through the application of this general method of simulating sampling surveys, it is straightforward to model a number of different sampling methods at each randomly selected house.

However, modelling the actual sample collection that is carried out at the selected houses, as characterised by the application of the single house model (grey component of Figure 3.12) will differ depending on sampling method as follows:

- *RDT* re-sampling: The collection of a repeat *RD*T sample is simulated for houses where the initial *RDT* sample result failed one or more of the prescribed lead standards. The simulated repeated sample is modelled in the same manner as *RDT* samples but at a second randomly selected time during the same daytime period.

- *30MS* sampling: The collection of a *1-litre* sample drawn after a *30-minute* stagnation period, which commences after the pipework has been fully flushed.

- *COMP* sampling: Sample concentration is set to the *DAC* computed for the house.

- *6-hour* stagnation sampling: The collection of a *1-litre* sample drawn after a *6-hour* stagnation period, which commences after the pipework has been fully flushed (with reference to US-EPA lead rule).

As with *RDT* sampling, the sample concentration computed for each house is compared to a number of lead standards, such as *10μg/l*, *25μg/l*, and *50μg/l*, and zonal failure rates, i.e. the percentage of houses in the zone where the sample concentration exceeds these standards are computed. However, in the case of *6-hour* stagnation sampling, the US-EPA standard for lead in drinking water is set as *15μg/l* at the 90th percentile.

Statistics such as mean and standard deviation of the number of samples in a survey that fail at each water quality standard are also computed.

3.2.5 FORTRAN implementation

The primary objective of this research, from a zonal perspective, was to develop a computational model, to be used by water engineers, to assess zonal compliance and facilitate the optimisation of corrective treatment. In order to incorporate the flexibility to assess a wide range of zonal scenarios, the model for generating a zone and simulating compliance assessment across a zone has been implemented in a computer program, developed using FORTRAN. This 'zonal program' is coupled to the 'house program', previously discussed (Chapter 2.2.6), since compliance assessment relies on the modelling of lead emissions at a single house. Unifying these two programs also facilitates subsequent modifications and provides a more convenient 'all in one' solution.

3.2.5.1 Input for zone generation

Parameters required to generate and subsequently store a complete description of a water supply zone include the size of the zone and the distribution of various household parameters:

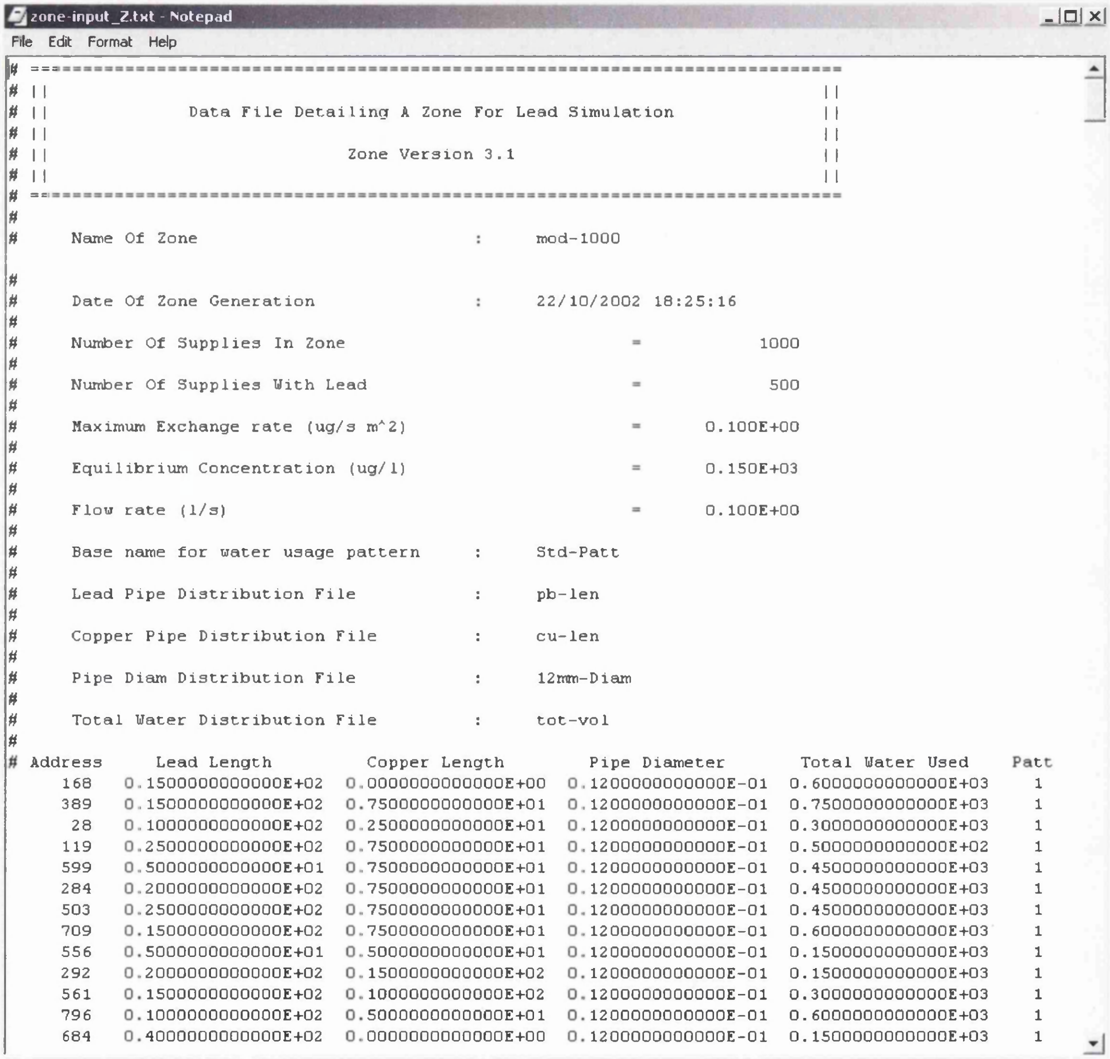
- General properties
    - Size of zone (total number of houses)
    - Percentage of houses supplied through lead pipework

- Household parameters
    - Length of Lead Pipework (distribution)
    - Length of Copper Pipework (distribution)
    - Diameter of Pipework (distribution)
    - Total Daily Volume of Water Used (distribution)
    - Pattern of Water Usage (distribution)
    - Plumbosolvency parameters (distribution or constant)
    - Flow Rate (constant)

Distributions of household parameters are stored in discrete format, as previously discussed (Chapter 3.2.1), using data files, which can be edited, where appropriate, to facilitate best possible calibration to real-world zones.

A complete zonal data file, which stores household properties for every single house in the zone, is automatically generated upon input of the general zonal properties, constants and filenames specifying the distribution data files. Input of this data can be carried out, either through a data file or directly by the user through the software's text menu system. The actual process of automatic zone generation is carried out through the application of the Monte Carlo method as previously discussed and is characterised by Figure 3.10.

The zonal data file generated includes a quantity of header information, which includes details such as the date that the zone was generated, general zonal properties, constants and the filenames specifying the distribution data files used (Figure 3.13). Subsequent data describes household characteristics of every single house in the zone and is stored in the form of a list of houses with corresponding household parameters, as characterised by Eqn. 3.2.



```
# ===========================================================================
# ||                                                                       ||
# ||              Data File Detailing A Zone For Lead Simulation           ||
# ||                                                                       ||
# ||                          Zone Version 3.1                             ||
# ||                                                                       ||
# ===========================================================================
#
#      Name Of Zone                          :     mod-1000

#
#      Date Of Zone Generation               :     22/10/2002 18:25:16
#
#      Number Of Supplies In Zone                          =          1000
#
#      Number Of Supplies With Lead                        =           500
#
#      Maximum Exchange rate (ug/s m^2)                    =     0.100E+00
#
#      Equilibrium Concentration (ug/l)                    =     0.150E+03
#
#      Flow rate (l/s)                                     =     0.100E+00
#
#      Base name for water usage pattern     :     Std-Patt
#
#      Lead Pipe Distribution File           :     pb-len
#
#      Copper Pipe Distribution File         :     cu-len
#
#      Pipe Diam Distribution File           :     12mm-Diam
#
#      Total Water Distribution File         :     tot-vol
#
# Address     Lead Length         Copper Length        Pipe Diameter        Total Water Used     Patt
     168   0.150000000000E+02  0.000000000000E+00  0.120000000000E-01  0.600000000000E+03    1
     389   0.150000000000E+02  0.750000000000E+01  0.120000000000E-01  0.750000000000E+03    1
      28   0.100000000000E+02  0.250000000000E+01  0.120000000000E-01  0.300000000000E+03    1
     119   0.250000000000E+02  0.750000000000E+01  0.120000000000E-01  0.500000000000E+02    1
     599   0.500000000000E+01  0.750000000000E+01  0.120000000000E-01  0.450000000000E+03    1
     284   0.200000000000E+02  0.750000000000E+01  0.120000000000E-01  0.450000000000E+03    1
     503   0.250000000000E+02  0.750000000000E+01  0.120000000000E-01  0.450000000000E+03    1
     709   0.150000000000E+02  0.750000000000E+01  0.120000000000E-01  0.600000000000E+03    1
     556   0.500000000000E+01  0.500000000000E+01  0.120000000000E-01  0.150000000000E+03    1
     292   0.200000000000E+02  0.150000000000E+02  0.120000000000E-01  0.150000000000E+03    1
     561   0.150000000000E+02  0.100000000000E+02  0.120000000000E-01  0.300000000000E+03    1
     796   0.100000000000E+02  0.500000000000E+01  0.120000000000E-01  0.600000000000E+03    1
     684   0.400000000000E+02  0.000000000000E+00  0.120000000000E-01  0.150000000000E+03    1
```

Figure 3.13. Zonal data file.

If desired, a zonal data file can be edited manually, which may be required when 'fine tuning' to very small water supply zones or performing small zonal investigations.

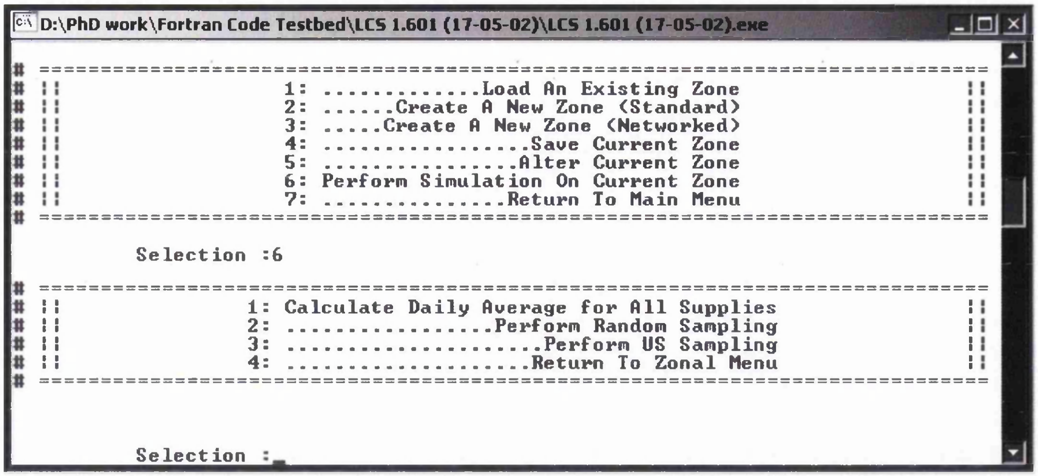
The capability to save, load and alter detailed descriptions of complete water supply zones allows greater flexibility when investigating the likely effects of plumbosolvency control on a zone as well as allowing the user to precisely specify zonal circumstances. Due to this flexible approach, a simulated zone can be retained for subsequent repetitive investigations of the results from simulated sampling exercises. Additionally, a detailed description of the simulated water supply zone will allow greater understanding of the likely characteristics of problem properties, where lead emissions will be highest.

3.2.5.2 Input for compliance assessment

The input required to simulate compliance assessment on a previously generated zonal data file include the specific details of the method of compliance assessment:

- Zonal data file
- Type of compliance assessment (Exact assessment / RDT sampling / US-EPA sampling)
- For sampling simulations:
    - Number of samples in a survey
    - Number of surveys to perform
- Water Quality Standard (i.e. a standard for lead in drinking water, such as *10*, *25* or *50μg/l*)
- Output options (Full data / Summary only)

These options are input into the model, by the user, through the software's text menu system (Figure 3.14). Additionally, the user is asked to specify the flow model and the mass transfer model that will be used since compliance assessment relies on the modelling of lead emissions at a single house.



```
# ============================================================================
# !!                  1: .............Load An Existing Zone                    !!
# !!                  2: ......Create A New Zone (Standard)                    !!
# !!                  3: .....Create A New Zone (Networked)                    !!
# !!                  4: .................Save Current Zone                    !!
# !!                  5: ................Alter Current Zone                    !!
# !!                  6: Perform Simulation On Current Zone                    !!
# !!                  7: ...............Return To Main Menu                    !!
# ============================================================================

         Selection :6

# ============================================================================
# !!               1: Calculate Daily Average for All Supplies                 !!
# !!               2: .................Perform Random Sampling                 !!
# !!               3: .....................Perform US Sampling                 !!
# !!               4: ....................Return To Zonal Menu                 !!
# ============================================================================


         Selection :_
```

Figure 3.14. User options within the software.

3.2.5.3 General algorithm

The FORTRAN code that has been developed to simulate compliance assessment of a previously generated zonal data file is capable of computing a range of valuable summary statistics, including failure rates for specific lead standards. In the case of the exact assessment simulation, the code is characterised by the general algorithm:

```
USER INPUT
  • Zonal data file
  • Flow and Mass transfer model
  • Water quality standards

EXACT ASSESSMENT
  • Read in all zonal data
  • For every house in the zone ($k = 1,H^T$)
        If house does not have lead pipework:
          o Set $DAC = 0$, $30MS = 0$, $Time = 0$
          o Output: Data for house:
              ▪ Household parameters and DAC, 30MS, Time results for house
        If house does have lead pipework:
          o Run single house model
              ▪ Compute: DAC
              ▪ Compute: Total time water quality standard is exceeded in 24-hour day
          o Simulate 30-minute stagnation test
              ▪ Compute 30MS sample concentration
          o Check to see if DAC exceeds water quality standards
          o Check to see if 30MS exceeds water quality standards
          o Compute (& Output): Data for house:
              ▪ Household parameters and DAC, 30MS, Time results for house
  • Next house
  • Compute (& Output): Summary data (zonal failure rates):
      o Percentage of houses where DAC exceeds water quality standards
      o Percentage of houses where 30MS exceeds water quality standards
```

Figure 3.15. General algorithm for simulation of exact assessment.

In the case of the sampling simulation, the code is characterised by the general algorithm:

```
USER INPUT
• Zonal data file
• Sampling scheme
    o Number of samples in each survey, n
    o Number of surveys to perform, m
• Flow and Mass transfer model
• Water quality standards

SAMPLING
• Read in all zonal data

• For every survey (k = 1,m)

    • For every sample (l = 1,n)

        o Randomly select house
        o If house does not use water between 9am and 5pm:
            ▪ Randomly select a different house

        If house does not have lead pipework:

        o Set DAC = 0, 30MS = 0, Time = 0
        o Output: Data for house:
            ▪ Household parameters and DAC, 30MS, Time results for house

        If house does have lead pipework:

        o Randomly select sampling time ST
        o Run single house model until ST
        o Simulate collection of a 1-litre sample
            ▪ Compute RDT sample concentration
        o Check to see if RDT exceeds water quality standards

        o If RDT exceeds any water quality standard
            ▪ Randomly select a new sampling time ST
            ▪ Run single house model until ST
            ▪ Simulate collection of a 1-litre sample
                • Compute RDT sample concentration
            ▪ Check to see if RDT exceeds water quality standards

        o Run single house model
            ▪ Compute: DAC
            ▪ Compute: Total time water quality standard is exceeded in 24-hour day
        o Simulate 30-minute stagnation test
            ▪ Compute 30MS sample concentration
        o Check to see if DAC exceeds water quality standards
        o Check to see if 30MS exceeds water quality standards

    • Next sample

    • Compute (& Output): Data for survey:
        o Number of samples that exceed water quality standards for:
            ▪ RDT, RDT-resample, 30MS, DAV
• Next survey

• Compute (& Output): Summary data (zonal failure rates):
    o Average percentage of samples that exceed water quality standards for:
        ▪ RDT, RDT-resample, 30MS, DAV
• Compute (& Output): Summary statistics:
    o Mean, Standard deviation, Minimum, Maximum of survey results for:
        ▪ RDT, RDT-resample, 30MS, DAV
• Compute (& Output): Confidence Limits for the percentage of samples that exceed each water quality standard
  for RDT
```

Figure 3.16. General algorithm for simulation of sampling.

3.2.5.4 Parallelisation

The computer programs described herein have been primarily developed to suit the needs of a water engineer having limited computing resources, i.e. will have access to a standard PC rather than a supercomputer. Indeed, through the use of the simple plug flow – exponential model to simulate household lead emissions, it is possible to perform large zonal simulations. However, in order to fully investigate very large zonal problems using the more complex fluid flow and mass transfer models, such as turbulent – diffusion model, in a reasonable timeframe very fast processing capabilities are required. Such processing capabilities can only be found in the form of:

- Supercomputers: typically comprise *4* or more individual CPUs (Central Processing Units) that run independently, i.e. has a parallel architecture.
- A number of individual computers that are connected to a computer network system.

In order to take advantage of these computing resources, i.e. those that have multiple CPUs, such as the *32*-processor SGI Onyx that has been available during this work, a parallelised version of the computer program has been developed. Parallelisation enables a single program to function across multiple CPUs. This was achieved by modifying the existing FORTRAN code to enable small independent sections of the complete zonal simulation to be assigned to different CPUs.

The most convenient method of dicretising zonal simulations across the available computing resources is to simply assign each 'slave' CPU (these are specified by the user) a house that requires evaluation in terms of *RDT* or *DAC*, depending on the method of compliance assessment. This process of delegation is carried out by a 'master' CPU (this is specified by the user). The 'master' and 'slave' CPUs communicate through MPI (Message Passing Interface) subroutines and libraries, which manage the transfer of data between instances of a parallel program running on multiple CPUs in a parallel computing architecture. Essentially the 'master' CPU manages the 'slave' CPUs and collates the results, while the 'slave' CPUs run the code, characterised by the highlighted sections of Figure 3.15 and Figure 3.16 for exact assessment and sampling simulations respectively.

Communication within the parallelised program during simulation of zonal assessment is illustrated for a configuration having *5* processors (Figure 3.17), where the connecting arrows represent the transfer of data (illustrated in grey), through MPI.

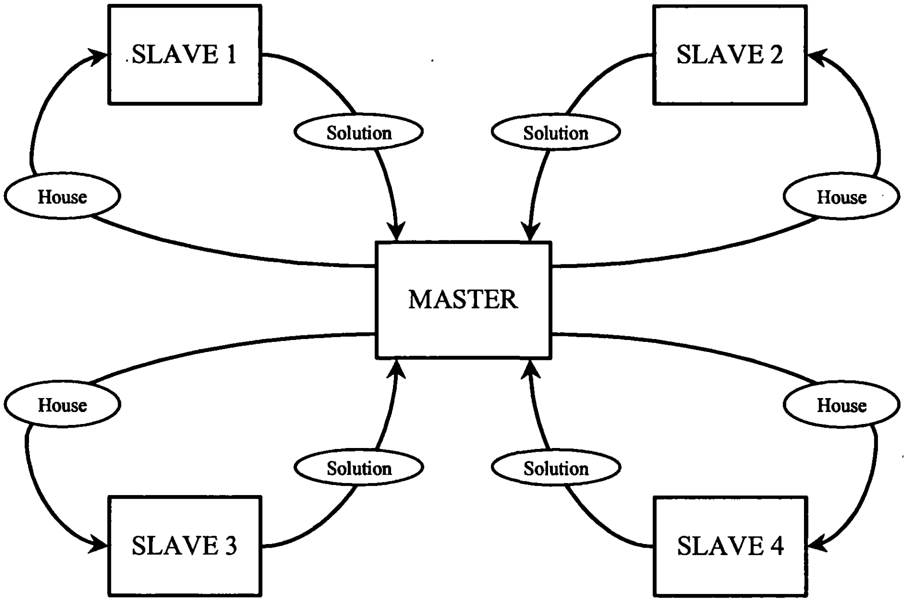


Figure 3.17. Communication within the parallelised program.

The development of a parallelised version of the computer program has enabled very large zonal problems to be investigated much faster than would be possible with the single-processor version of the computer program. As an example, processing times are given in Table 3.1 for a *DAC* simulation using the turbulent – diffusion model on a zone having approximately *16,000* houses with lead pipes.

Table 3.1. Processing time for large zonal simulation.

Version of Program	Computing Platform	Processing Time (hr)
Single-Processor	Pentium III 600 MHz	33
Parallel	SGI Onyx (using 20 out of 32 processors)	0.5

3.2.5.5 Output for exact assessment of compliance

The output produced for a simulation of exact assessment of zonal compliance includes summary data for every single house in the zone that relate to lead emissions computed for one day, as well as summary data for the zone as a whole:

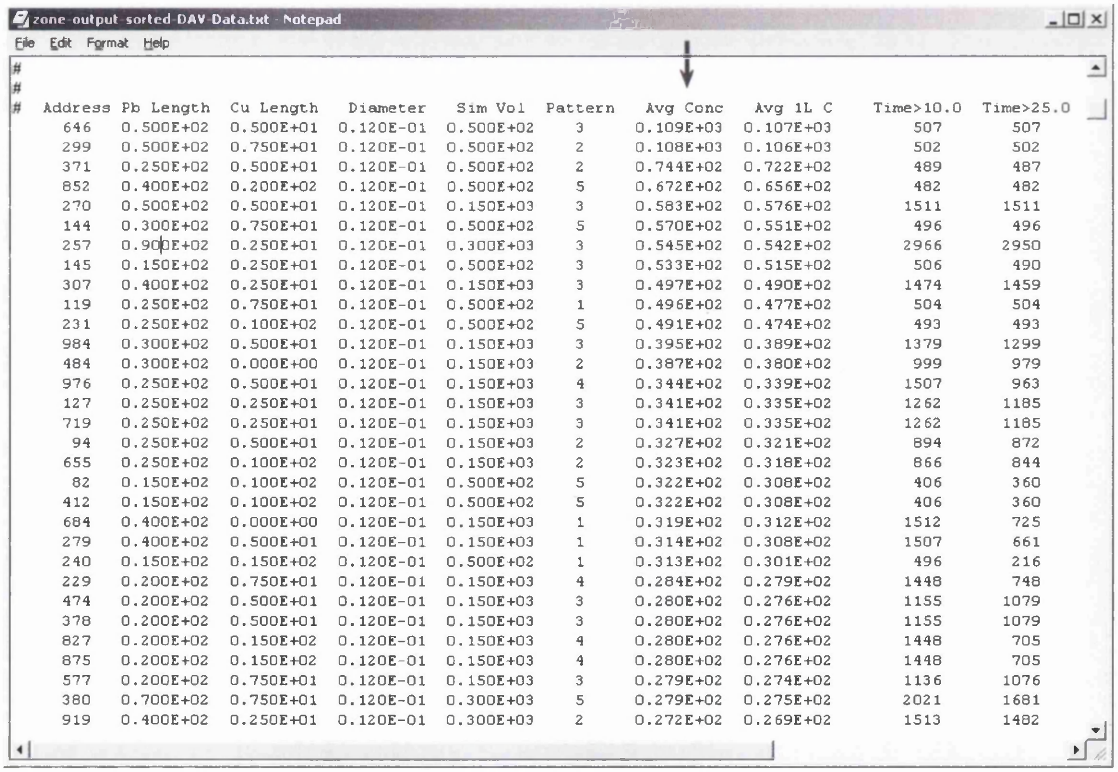
- For every house in the zone, the following are output:
    - Household parameters
    - *DAC*

  - *30MS*
  - Total time each water quality standard is exceeded in the 24-hour simulation period

- For the zone as a whole, the following are output:
  - Percentage of houses that fail each water quality standard, based on *DAC*
  - Percentage of houses that fail each water quality standard, based on *30MS*
  - Time taken for computer to process the entire simulation

Summary data for each house within the zone is output as a new row within a 'zonal data' file, similar in form to the zonal data file, though with additional entries for *DAC*, *30MS* and total time each water quality standard is exceeded in the 24-hour simulation period (Figure 3.18).

Additionally, a feature within the software allows the user to specify whether to sort the houses by descending *DAC* on output (indicated within Figure 3.18) or to output houses in the same order as the zonal data file. Sorting the houses by descending *DAC* allows greater understanding of the likely characteristics of problem properties, where lead emissions will be highest.

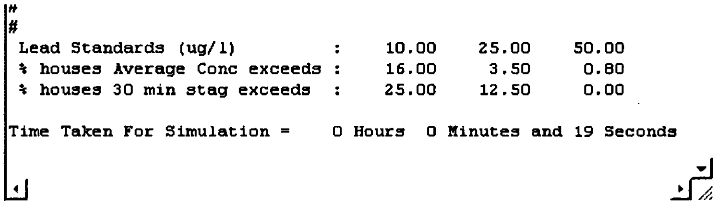


```
#
#
#  Address Pb Length  Cu Length   Diameter   Sim Vol  Pattern   Avg Conc   Avg 1L C     Time>10.0  Time>25.0
     646  0.500E+02  0.500E+01  0.120E-01  0.500E+02     3     0.109E+03  0.107E+03       507        507
     299  0.500E+02  0.750E+01  0.120E-01  0.500E+02     2     0.108E+03  0.106E+03       502        502
     371  0.250E+02  0.500E+01  0.120E-01  0.500E+02     2     0.744E+02  0.722E+02       489        487
     852  0.400E+02  0.200E+02  0.120E-01  0.500E+02     5     0.672E+02  0.656E+02       482        482
     270  0.500E+02  0.500E+01  0.120E-01  0.150E+03     3     0.583E+02  0.576E+02      1511       1511
     144  0.300E+02  0.750E+01  0.120E-01  0.500E+02     5     0.570E+02  0.551E+02       496        496
     257  0.900E+02  0.250E+01  0.120E-01  0.300E+03     3     0.545E+02  0.542E+02      2966       2950
     145  0.150E+02  0.250E+01  0.120E-01  0.500E+02     3     0.533E+02  0.515E+02       506        490
     307  0.400E+02  0.250E+01  0.120E-01  0.150E+03     3     0.497E+02  0.490E+02      1474       1459
     119  0.250E+02  0.750E+01  0.120E-01  0.500E+02     1     0.496E+02  0.477E+02       504        504
     231  0.250E+02  0.100E+02  0.120E-01  0.500E+02     5     0.491E+02  0.474E+02       493        493
     984  0.300E+02  0.500E+01  0.120E-01  0.150E+03     3     0.395E+02  0.389E+02      1379       1299
     484  0.300E+02  0.000E+00  0.120E-01  0.150E+03     2     0.387E+02  0.380E+02       999        979
     976  0.250E+02  0.500E+01  0.120E-01  0.150E+03     4     0.344E+02  0.339E+02      1507        963
     127  0.250E+02  0.250E+01  0.120E-01  0.150E+03     3     0.341E+02  0.335E+02      1262       1185
     719  0.250E+02  0.250E+01  0.120E-01  0.150E+03     3     0.341E+02  0.335E+02      1262       1185
      94  0.250E+02  0.500E+01  0.120E-01  0.150E+03     2     0.327E+02  0.321E+02       894        872
     655  0.250E+02  0.100E+02  0.120E-01  0.150E+03     2     0.323E+02  0.318E+02       866        844
      82  0.150E+02  0.100E+02  0.120E-01  0.500E+02     5     0.322E+02  0.308E+02       406        360
     412  0.150E+02  0.100E+02  0.120E-01  0.500E+02     5     0.322E+02  0.308E+02       406        360
     684  0.400E+02  0.000E+00  0.120E-01  0.150E+03     1     0.319E+02  0.312E+02      1512        725
     279  0.400E+02  0.500E+01  0.120E-01  0.150E+03     1     0.314E+02  0.308E+02      1507        661
     240  0.150E+02  0.150E+02  0.120E-01  0.500E+02     1     0.313E+02  0.301E+02       496        216
     229  0.200E+02  0.750E+01  0.120E-01  0.150E+03     4     0.284E+02  0.279E+02      1448        748
     474  0.200E+02  0.500E+01  0.120E-01  0.150E+03     3     0.280E+02  0.276E+02      1155       1079
     378  0.200E+02  0.500E+01  0.120E-01  0.150E+03     3     0.280E+02  0.276E+02      1155       1079
     827  0.200E+02  0.150E+02  0.120E-01  0.150E+03     4     0.280E+02  0.276E+02      1448        705
     875  0.200E+02  0.150E+02  0.120E-01  0.150E+03     4     0.280E+02  0.276E+02      1448        705
     577  0.200E+02  0.750E+01  0.120E-01  0.150E+03     3     0.279E+02  0.274E+02      1136       1076
     380  0.700E+02  0.750E+01  0.120E-01  0.300E+03     5     0.279E+02  0.275E+02      2021       1681
     919  0.400E+02  0.250E+01  0.120E-01  0.300E+03     2     0.272E+02  0.269E+02      1513       1482
```

Figure 3.18. Output data for exact assessment of compliance.

Summary data for the zone as a whole is output within a 'zonal summary' file, with entries for zonal failure rates at each water quality standard for both *DAC* and *30MS* (Figure 3.19).

Furthermore, it is possible to output a range of highly detailed data for each house in the zone, such as the concentration in each element of the pipework for every second throughout the 24-hour simulation period, as previously discussed (Chapter 2.2.6.3).



```
#
#
 Lead Standards (ug/l)          :    10.00    25.00    50.00
 % houses Average Conc exceeds  :    16.00     3.50     0.80
 % houses 30 min stag exceeds   :    25.00    12.50     0.00

Time Taken For Simulation =    0 Hours  0 Minutes and 19 Seconds
```

Figure 3.19. Output summary for exact assessment of compliance.

3.2.5.6 Output for simulation of multiple RDT sampling surveys

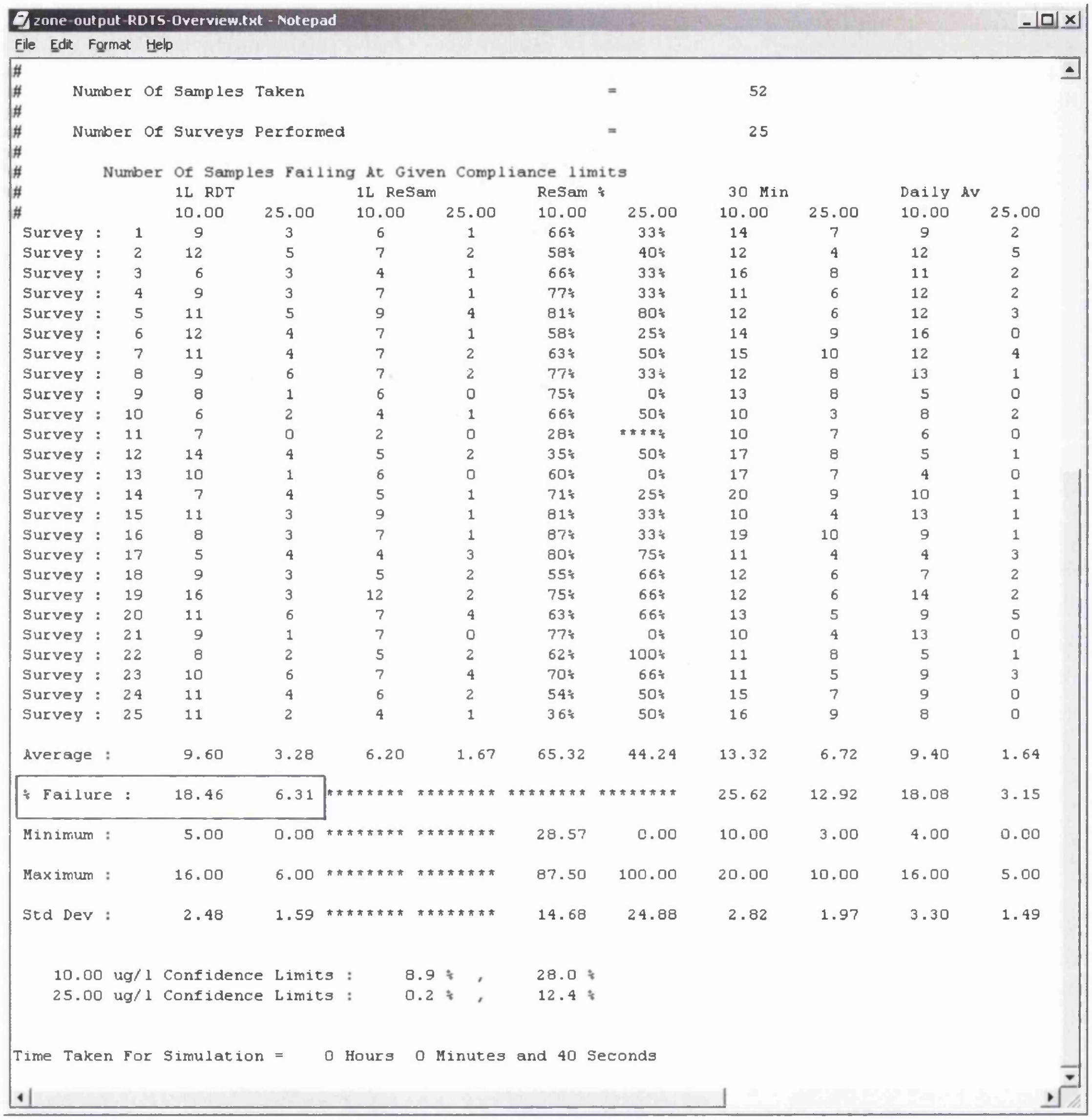
The output produced for a simulation of multiple *RDT* sampling surveys includes summary data for every single sampling survey simulated, as well as summary statistics for all surveys:

- For every survey performed, the following are output:
    - Number of samples in survey that fail each water quality standard, based on:
        - *RDT* sample concentration
        - *RDT* re-sample concentration
        - *30MS* sample concentration
        - *DAC*

- The following summary statistics based on data from all surveys performed are output:
    - Mean failure rate as well as the mean, minimum, maximum and standard deviation of the number of samples in survey that fail each water quality standard, based on:
        - *RDT* sample concentration
        - *RDT* re-sample concentration
        - *30MS* sample concentration
        - *DAC*
    - Upper and lower confidence limits for the Mean *RDT* failure rate

  - Time taken for computer to process the entire simulation

Summary data for each survey simulated within the zone is output as a new row within a ‘sampling output’ data file (Figure 3.20). This is followed by the summary statistics for all surveys simulated, as detailed above.



```
#
#     Number Of Samples Taken                              =             52
#
#     Number Of Surveys Performed                          =             25
#
#        Number Of Samples Failing At Given Compliance limits
#               1L RDT            1L ReSam          ReSam %           30 Min            Daily Av
#               10.00    25.00    10.00    25.00    10.00    25.00    10.00    25.00    10.00    25.00
 Survey :   1     9        3        6        1       66%      33%      14        7        9        2
 Survey :   2    12        5        7        2       58%      40%      12        4       12        5
 Survey :   3     6        3        4        1       66%      33%      16        8       11        2
 Survey :   4     9        3        7        1       77%      33%      11        6       12        2
 Survey :   5    11        5        9        4       81%      80%      12        6       12        3
 Survey :   6    12        4        7        1       58%      25%      14        9       16        0
 Survey :   7    11        4        7        2       63%      50%      15       10       12        4
 Survey :   8     9        6        7        2       77%      33%      12        8       13        1
 Survey :   9     8        1        6        0       75%       0%      13        8        5        0
 Survey :  10     6        2        4        1       66%      50%      10        3        8        2
 Survey :  11     7        0        2        0       28%   *****%      10        7        6        0
 Survey :  12    14        4        5        2       35%      50%      17        8        5        1
 Survey :  13    10        1        6        0       60%       0%      17        7        4        0
 Survey :  14     7        4        5        1       71%      25%      20        9       10        1
 Survey :  15    11        3        9        1       81%      33%      10        4       13        1
 Survey :  16     8        3        7        1       87%      33%      19       10        9        1
 Survey :  17     5        4        4        3       80%      75%      11        4        4        3
 Survey :  18     9        3        5        2       55%      66%      12        6        7        2
 Survey :  19    16        3       12        2       75%      66%      12        6       14        2
 Survey :  20    11        6        7        4       63%      66%      13        5        9        5
 Survey :  21     9        1        7        0       77%       0%      10        4       13        0
 Survey :  22     8        2        5        2       62%     100%      11        8        5        1
 Survey :  23    10        6        7        4       70%      66%      11        5        9        3
 Survey :  24    11        4        6        2       54%      50%      15        7        9        0
 Survey :  25    11        2        4        1       36%      50%      16        9        8        0

 Average :       9.60     3.28     6.20     1.67    65.32    44.24    13.32     6.72     9.40     1.64

 % Failure :    18.46     6.31 ******** ******** ******** ********    25.62    12.92    18.08     3.15

 Minimum :       5.00     0.00 ******** ********    28.57     0.00    10.00     3.00     4.00     0.00

 Maximum :      16.00     6.00 ******** ********    87.50   100.00    20.00    10.00    16.00     5.00

 Std Dev :       2.48     1.59 ******** ********    14.68    24.88     2.82     1.97     3.30     1.49


    10.00 ug/l Confidence Limits :     8.9 %  ,     28.0 %
    25.00 ug/l Confidence Limits :     0.2 %  ,     12.4 %


Time Taken For Simulation =    0 Hours  0 Minutes and 40 Seconds
```

Figure 3.20. Output for simulation of multiple RDT sampling surveys.

3.3 Results for a water supply zone

3.3.1 Introduction

Through the application of the mathematics of mass transfer and fluid flow, lead emissions at a single property have been modelled in great detail. This has facilitated the study of the influence of household parameters, such as pipework and water usage, on lead emissions. However, in order to understand the general issues that relate to plumbosolvency control on a zonal scale, it is necessary to investigate the zonal variation of lead emissions and the influence of zonal factors on compliance, in terms of both exact assessment and RDT sampling. This can be achieved through the employment of the zonal model, which can simulate the structure of an entire water supply zone and subsequent compliance assessment methodologies, as previously described (Chapter 3.2).

3.3.2 Zonal variation of lead emissions

3.3.2.1 Exact assessment

'Exact' assessment is the most comprehensive method of determining zonal compliance in accordance with the new directive and involves the characterisation of all lead emissions occurring across a zone during one simulated day. The primary output obtained from the simulation of exact assessment is the zonal failure rate for each lead standard, i.e. the percentage of houses where the *DAC* exceeds lead standards of *10μg/l*, *25μg/l*, and *50μg/l*.

Before compliance assessment can be simulated, a full description of a water supply zone must be generated. The average water supply zone in the U.K. contains approximately *10,000 houses*, *40%* of which having lead pipework. However, in order to minimise computation time, it is sufficient to represent an 'average' zone using *2,000 houses*, *40%* of which having lead pipework. This has been justified by the results of sensitivity analyses of the effect of zone size on both *DAC* and *RDT* simulation results (Chapter 3.4). The parameters used to generate such a zone are given the following values:

- General properties
    - Size of zone: *2000 houses*
    - Houses with lead pipework: *40%*

- Household parameters

- Length of lead pipework: standard distribution (Figure 3.3)
- Length of copper pipework: standard distribution (Figure 3.4)
- Diameter of pipework: *12mm*
- Total daily volume of water used: standard distribution (Figure 3.6)
- Pattern of water usage: equal application of *5* different patterns (Chapter 3.2.1.3)
- Plumbosolvency parameters:
  - Equilibrium concentration, *E*: *150μg/l*
  - Initial mass transfer rate, *M*: $0.1 \mu g/m^2/s$
  - Diffusion coefficient, *D*: $4.96E\text{-}10 m^2/se$
- Flow rate: *0.1l/s*

It is likely that the flow within a pipe for typical residential use is turbulent, since the flow rate is approximately *0.1l/s* under normal use, which translates to a Reynolds number greater than *9000*. Consequently, solutions of compliance assessment will be obtained from the model for turbulent flow. These will be compared to the equivalent solutions from the simpler plug flow model. In the case of the turbulent flow model, solutions from both diffusion model and exponential approximation of mass transfer can be obtained. However, in the case of the plug flow model, only the exponential approximation is used.

Compliance assessment, based on *DAC* (exact assessment) at the *10*, *25* and *50μg/l* standards, was carried out on the 'average' zone, previously generated. The solutions illustrate that the failure rates based on *DAC* are significantly higher at the more stringent lead standard of *10μg/l* than for the *25* and *50μg/l* standards (Figure 3.21).

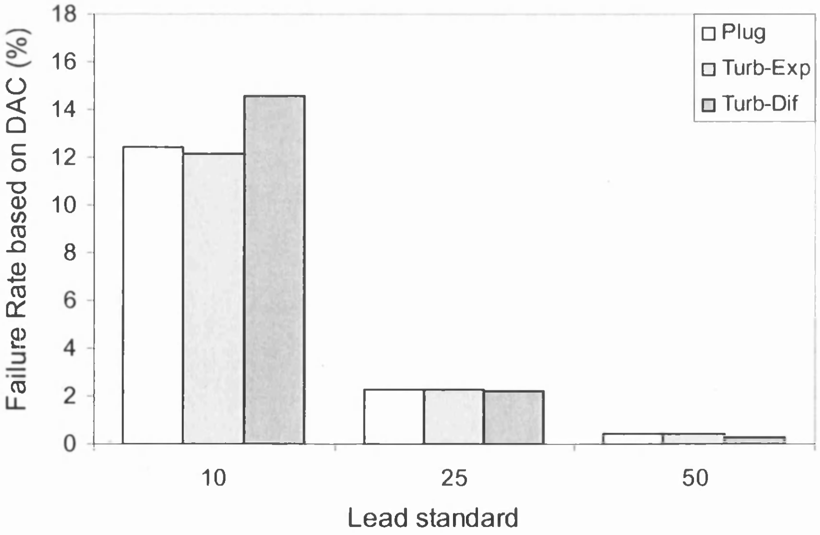


Figure 3.21. Solutions of exact compliance assessment.

Failure rates will always be higher at the more stringent standards because they inherently include the failure rate at the next standard. However, it is observed that failure rates between the *10* and *25μg/l* standards (the difference between the failure rate at *10μg/l* and the failure rate at *25μg/l*) are significantly greater than those between the *25* and *50μg/l* standards.

This also illustrates the similarity in results from each computational model at each lead standard. The failure rates based on *DAC* computed using the exponential model, i.e. plug flow and turbulent – exponential models, are virtually identical across all three lead standards. This is essentially because the *DAC* of a house is primarily governed by the mass transfer model as opposed to the flow model; a result of the principal of conservation of mass. When the more sophisticated 'diffusion model' is used to simulate mass transfer, slightly different failure rates are observed. In particular, failure rates become more skewed towards the more stringent lead standards. This is because the mass transfer rate during stagnation for high initial concentrations, which will often occur at houses that fail the less stringent standards, is higher in the case of the exponential model.

The zonal model incorporates the flexibility to output summary data for every single house in the zone that relate to lead emissions computed for one day, as well as summary data for the zone as a whole. This enables the full variation in lead emissions that occurs across the simulated zone to be quantified and allows greater understanding of the likely characteristics of problem properties, where lead emissions will be highest.

DAC of houses within the zone that have lead pipework is illustrated for each model (Figure 3.22). Note that this plot omits results for houses without a lead pipe, i.e. *60%* houses having a *DAC* of zero, as this is deemed unnecessary.

Figure 3.22 clearly illustrates how, for each model, the proportion of houses decreases rapidly with increasing *DAC*, i.e. the histograms are skewed towards low *DAC*. This is because the factors that increase *DAC,* such as increasing lead pipework length, become progressively less probable as defined by the distribution of that parameter, e.g. it is very unlikely that a house will have *90m* of lead pipework. Extremely high *DAC* may be caused by a combination of several factors, such as very long lead pipework in conjunction with very low daily water consumption, though the probability is extremely small. Indeed, for each model, the highest *DAC*, by a considerable margin, is observed for a house having *40m* of lead pipework and a daily water consumption of *50l.*

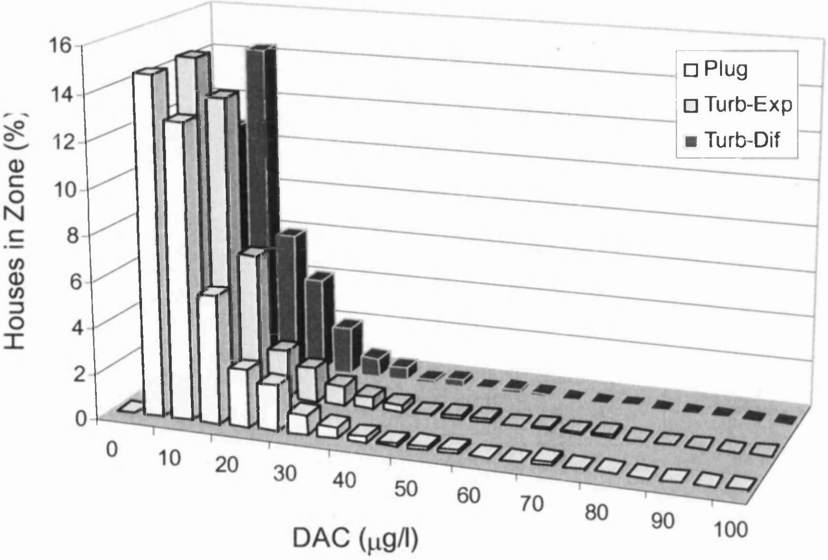


Figure 3.22. Histogram of the DAC of houses in zone.

From the analysis of these output data, several statistical parameters have been found; these reveal more subtle differences between the results from each model (Table 3.2).

Table 3.2. Statistical properties of DAC of houses that have lead pipework.

	Plug	**Turb-Exp**	**Turb-Dif**
Mean	9.7	9.4	10.4
Median	6.8	6.6	8.0
Minimum	1.0	0.9	1.1
Maximum	99.7	97.2	73.0
Standard Deviation	9.8	9.6	8.7

Note that the mean and median *DAC* for each model reflect the zonal failure rates at the *10μg/l* standard, previously illustrated (Figure 3.21). Also note that the maximum *DAC* observed is significantly lower when the more sophisticated 'diffusion model' is used to simulate mass transfer. This trend reflects zonal failure rates at the less stringent *25* and *50μg/l* standards, previously illustrated (Figure 3.21) and can be expected since the mass transfer rate during stagnation for high initial concentrations is higher in the case of the exponential model.

3.3.2.2 30 Minute Stagnation

In addition to *DAC*, the *30MS* test is simulated for every single house within the zone, resulting in zonal failure rates at each lead standard, i.e. the percentage of houses where the *30MS* sample concentration exceeds lead standards of *10μg/l*, *25μg/l*, and *50μg/l*. Once again, as expected, the solutions illustrate that the failure rates based on *30MS* are significantly higher at the more stringent lead standard of *10μg/l* than for the *25* and *50μg/l* standards (Figure 3.23). However, in the case of *30MS*, there are no failures at the *50μg/l* standard, since this concentration is not quite reached during the *30MS* test.

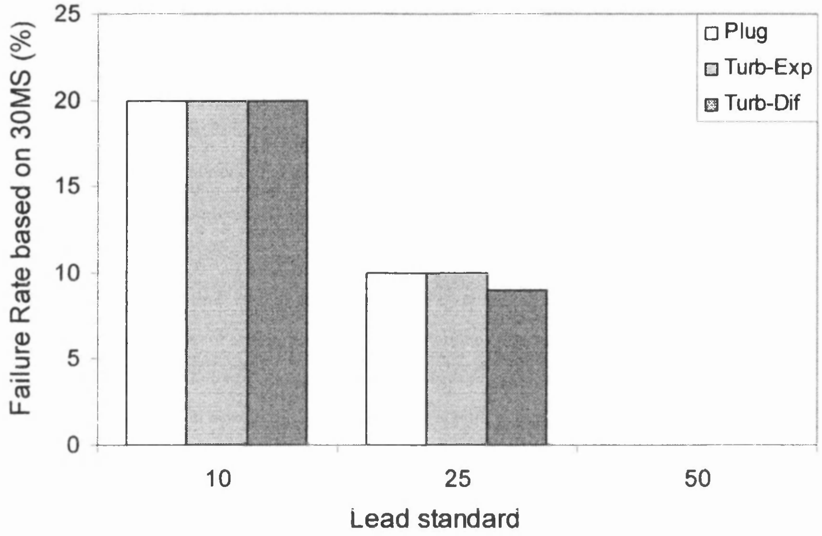


Figure 3.23. Solutions of 30MS compliance assessment.

The *30MS* sample concentration of houses within the zone that have lead pipework is illustrated for each model (Figure 3.24). Note that this plot effectively shows the *30MS* concentration at every house that has lead pipework within the zone as opposed to the number of houses that have a specific *30MS* concentration. The motivation for this is to illustrate that the *30MS* concentration will always be one of a relatively small number of possible concentrations.

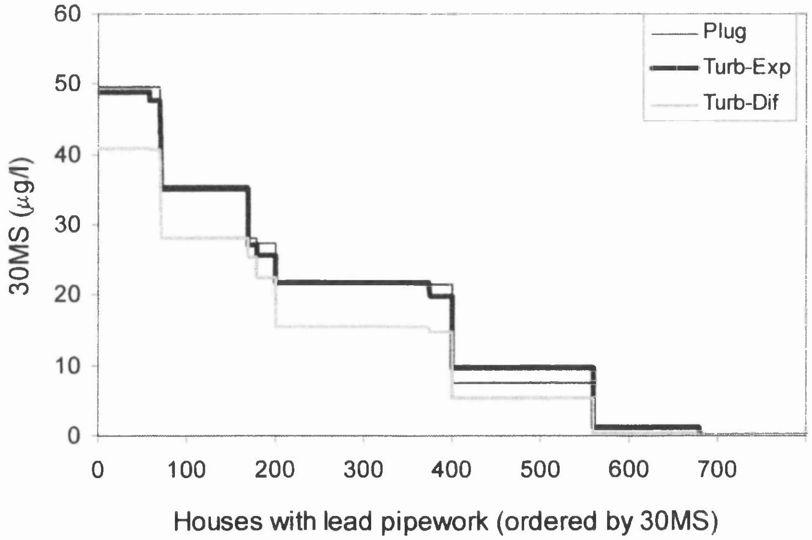


Figure 3.24. 30MS concentration of houses in zone.

This is because, for a zone having uniform plumbosolvency and pipework diameter, *30MS* concentration is a function of the length of lead pipework and the length of copper (non-lead) pipework only. Consequently, the limited number of different combinations of pipework lengths dictates the number of different *30MS* concentrations that can arise within a zone.

As previously demonstrated (Chapter 2.4.3.2), *30MS* concentration increases linearly with lead pipework length up to a length of *10m*, assuming a pipework diameter of *12mm*. However, *30MS* concentration decreases linearly with copper pipework length, a result of the dilution effect. Consequently, the maximum *30MS* concentration of observed within the zone is observed at houses having more than *10m* of lead pipework and no copper pipework. Similarly, a *30MS* concentration of zero is observed at houses having more than *10m* of copper pipework.

The solutions obtained from the diffusion model are consistently lower than the other models. This discrepancy can be explained by considering how the concentration varies across the pipe cross-section for each model of mass transfer during stagnation, as previously described (Chapter 2.3.1).

3.3.2.3 Duration of breach of water quality standards

In a similar manner to *30MS*, the duration that the *10μg/l*, *25μg/l*, and *50μg/l* lead standards are breached (during the simulated day) are plotted for houses within the zone that have lead pipework (Figure 3.25). In this example the plug flow model was used to simulate lead emissions.

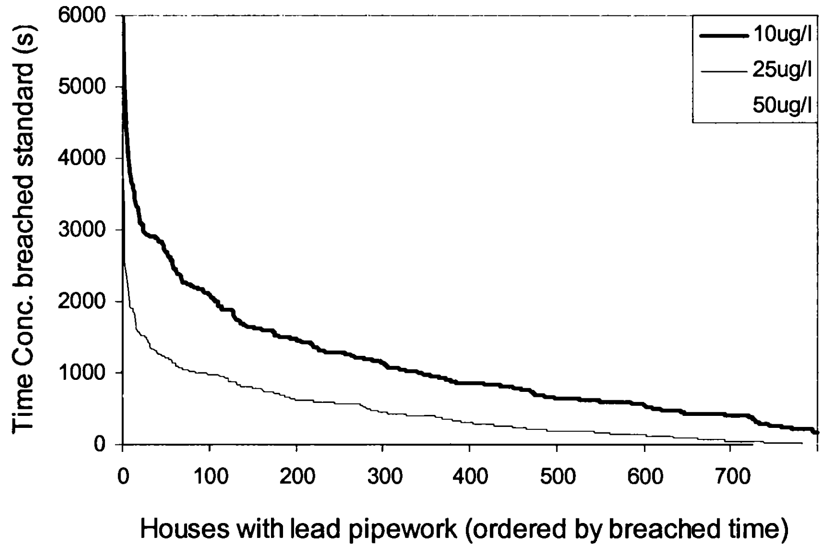


Figure 3.25. Duration that lead standards were breached in zone (Plug flow).

This clearly illustrates the fact that the less stringent standard of *50μg/l* is rarely breached. Indeed, even in the most extreme case, associated with a house having *80m* of lead pipework and a daily water consumption of *450l*, this standard is breached for just *700 secs* out of a total flow time of *4500 secs*, i.e. *16%* of the time. However, in the case of the house having the highest *DAC*, the *50μg/l* standard is breached for *484 secs* out of a total flow time of *500 secs*, i.e. *97%* of the time. It is found that only *16%* of houses in the zone that have lead pipework breach the *50μg/l* standard for more than one minute during the simulated day.

Conversely, it is found that the *10μg/l* standard is breached far more regularly since concentration within lead pipework after a typical stagnation period is usually in excess of *25μg/l* as defined by the stagnation curve for a moderately plumbosolvent water. It is found that all houses within the zone that have lead pipework breach the *10μg/l* standard for more than three minutes. Similar results are observed for the turbulent – exponential and turbulent – diffusion models.

3.3.3 RDT Sampling

The most widely used sampling technique, employed by water suppliers in the UK, is Random Day Time (*RDT*) sampling. This approach has been used extensively for assessing compliance with lead standards since 1989 and remains the most favoured protocol in terms of costs, practicality and consumer acceptance. Consequently, the ability of the zonal model to simulate *RDT* sampling is crucial for characterising the behaviour of a simulated zone in a way that can be validated to the real-world data collected by the water company. Additionally, output from the *RDT* sampling simulation will facilitate the investigation of reproducibility and possible variation in results of *RDT* sampling.

The simulated *RDT* sampling surveys to be carried out will comprises $n = 52$ samples in order to represent a typical *RDT* sampling survey, which is carried out over one year with one sample being taken from the water supply zone each week. However, since *RDT* sampling survey results are never completely reproducible the simulated survey will be repeated $m = 100$ times, in order to be able to understand possible variation.

The primary output obtained from the simulation of each *RDT* sampling survey is the number of samples that fail F^s for each water quality standard s, i.e. the number of samples where the concentration exceeds lead standards of *10μg/l*, *25μg/l*, and *50μg/l*. This data effectively forms a list of m values of F^s for each testing limit s, which can be thought of as a sample, of size *m*, from an infinitely large population. If *m* is sufficiently large (>*50*), the distribution of F^s can be assumed to be Normal.

The primary output obtained from the simulation of multiple sampling surveys are summary statistics based on data from all surveys performed. These include the mean $\overline{F}^s$ (Eqn. 3.4) and standard deviation σ^s (Eqn. 3.5) of the number of samples in a survey that fail for each water quality standard *s*. From these, the population estimates for the mean and standard deviation of the number of samples that fail F^s for each water quality standard *s*, are readily calculated as follows:

$$\hat{\overline{F}}^s = \overline{F}^s \qquad \text{Eqn. 3.6}$$

$$\hat{\sigma}^s = \sigma^s \sqrt{\frac{m}{m-1}} \qquad \text{Eqn. 3.7}$$

Estimates for the population parameters of the distribution of zonal failure rates in terms of percentages are calculated simply by dividing by the number of samples taken in each survey, *n* and multiplying by *100%*:

$$\hat{\overline{F}}^s\% = \hat{\overline{F}}^s \times 100/n \qquad \text{Eqn. 3.8}$$

$$\hat{\sigma}^s\% = \hat{\sigma}^s \times 100/n \qquad \text{Eqn. 3.9}$$

Before *RDT* sampling can be simulated, a full description of water supply zone must be generated. For initial investigation into the possible variation in results of *RDT* sampling, a simulated supply zone will be generated having the characteristics of an 'average' U.K. water supply zone. Consequently, the zone generated for the purposes of investigation of 'exact' assessment, previously described (Chapter 3.3.2) will be employed.

As in the case of 'exact' assessment, results from *RDT* sampling simulations will be obtained from the model for turbulent flow. These will be compared to the equivalent solutions from the simpler plug flow model. In the case of the turbulent flow model, solutions from both diffusion model and exponential approximation of mass transfer can be obtained. However, in the case of the plug flow model, only the exponential approximation is used.

3.3.3.1 Comparing solutions from *RDT* sampling to 'exact' assessment

A total of *100 RDT* sampling surveys were simulated on the 'average' zone, previously generated. The solution (Figure 3.26) reveals that, at the *25* and *50μg/l* standards, the mean zonal failure rate $\hat{\bar{F}}^{s}\%$ is significantly higher than the failure rate based on *DAC*, previously illustrated (Figure 3.21) for all three models. However, this trend is not observed at the *10μg/l* standard when the turbulent models are used, as failure rates based on *RDT* are not found to differ significantly from those based on *DAC*.

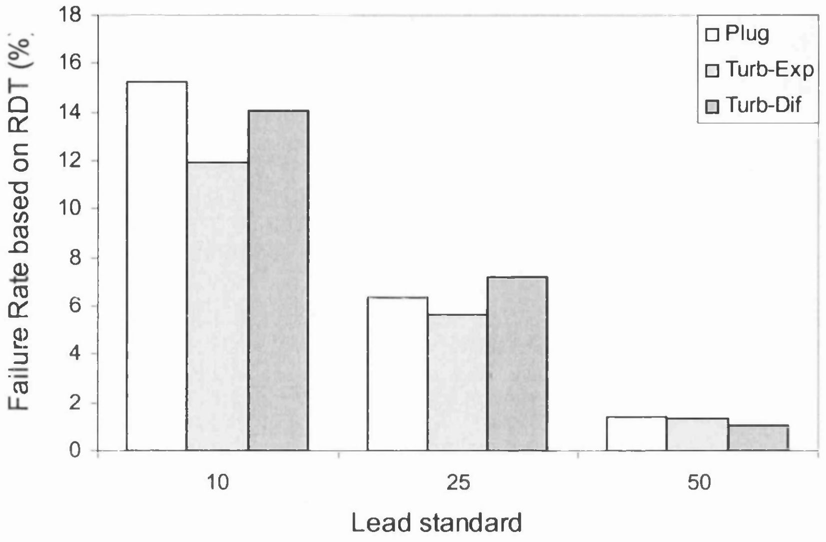


Figure 3.26. Solutions of RDT sampling compliance assessment.

The general trend of failure rates being higher when based on *RDT* suggests that, on average, the concentration of a one litre *RDT* sample taken from a house is greater than the *DAC* of that house; an observation consistent with other studies [22]. This is because, in general, *RDT* sample concentration is primarily a function of 'first draw' concentrations, whilst *DAC* is a function of both 'first draw' and 'steady state' concentrations (Figure 3.27) where:

- "First draw" concentrations:

High concentrations towards the start of the flow period caused by the lead that has dissolved into the water during the previous stagnation period.

- "Steady state" concentrations:

Low concentrations towards the end of the flow period arising when fresh water from the water main has flushed the majority of the dissolved lead from the pipe.

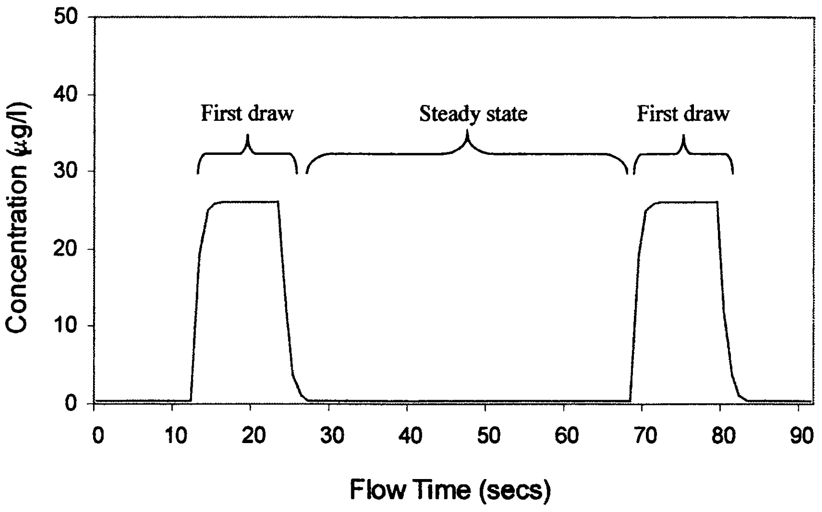


Figure 3.27. Concentration at the tap during flow.

However, *RDT* sample concentration will typically be lower than *DAC* when:

- The *RDT* sample is taken very soon after a flow period:
- The effective stagnation period before the sample is taken is very short, and hence the concentration within the lead pipework, which dictates the sample concentration, will be low in accordance with the stagnation curve.
- The house has long copper pipework between the tap and the lead pipework and high daily water consumption: As with *30MS* sample concentration, previously discussed (Chapter 2.4.3.3), *RDT* sample concentration decreases with length of copper pipework. This is because the *1-litre* sample, taken at the tap, will be comprised of water that has stagnated in the lead pipework, which will thus contain lead, as well as water that has stagnated within the copper pipework, which will contain a significantly lower concentration of lead. The proportion of water that has stagnated in the copper pipework is proportional to the length of copper pipework, thus determining the *RDT* sample concentration obtained.

3.3.3.2 Comparing solutions for each model

Solutions of zonal failure rates from the different mass transfer and flow models are observed to differ significantly more in the case of *RDT* than for *DAC*. In particular, solutions from the turbulent – exponential model are noticeably lower than those from the plug flow and turbulent – diffusion models.

This can partly be explained by considering the water usage involved in *RDT* sample collection. Although the time at which the sample is taken is randomly chosen, it is logical to assume that, on average, the sample will be taken during a stagnation period.

This is because the time for which water stagnates during the daytime far exceeds the time for which water is flowing. Additionally, it is logical to assume that for the average situation, the sample will be taken approximately halfway through a stagnation period, this being the average. Since the duration of the average stagnation period, as defined by the water usage patterns ascribed within the zone (Chapter 3.2.1.3), is *15 minutes*, it follows that the average 'effective' stagnation time before the *RDT* sample is taken, is equal to *7.5 minutes.*

Consequently, the concentration within the lead pipework will be significantly higher in the case of the diffusion model than for the exponential model since the initial rate of mass transfer is significantly higher, as previously described (Chapter 2.3.1). Assuming the pipework is sufficiently flushed during the previous flow period and the length of copper pipework is not greater than *2.5m*, the *RDT* sample concentration will be significantly higher, as represented by the difference in areas beneath the solutions between *0* and *10* seconds (Figure 3.28).

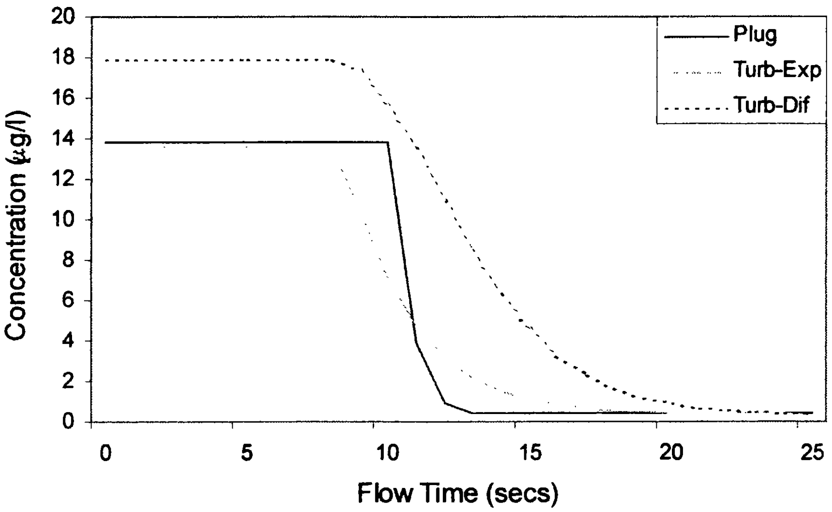


Figure 3.28. Concentration at tap after 7.5min stagnation (no Copper pipe).

In fact, a *RDT* sample taken after *7.5 minutes* 'effective' stagnation from a house having *2.5m* copper pipework is found to have a concentration greater than *10µg/l* when the diffusion model is used as opposed to a concentration less than *10µg/l* when the exponential model is used.

Solely considering this explanation accounts for the difference between failure rates for the turbulent - exponential and turbulent – diffusion models, though it does not explain why the failure rates from the plug – flow model are significantly higher than those from the turbulent – exponential model.

By deduction, this inconsistency must be a consequence of the difference between the plug and turbulent flow models. In particular, it is found that the limited boundary layer effects, which are observed in turbulent flow, result in a more gradual variation of concentration at the tap during flow. This smoother variation reduces the duration for which the maximum 'first draw' concentration is observed and in some cases will reduce the *RDT* sample concentration. This is caused by the 'flushing effect' that occurs in the middle of the pipe, where the fluid velocity is highest, as fresh water from the water main dilutes the leaded water, as previously described (Chapter 2.3.2.1). The effect is illustrated (Figure 3.28), where, for the turbulent flow model, the concentration of lead at the tap starts to decrease from the maximum 'first draw' concentration after *8 seconds* of flow, as opposed to *10 seconds* of flow for the plug flow model. Since a one-litre sample takes *10 seconds* to collect, it is clear that the sample concentration will be smaller in the case of turbulent flow, as represented by the difference in areas beneath the solutions between *0* and *10* seconds.

3.3.3.3 Variation of RDT sampling results

In addition to plotting the mean *RDT* failure rate $\hat{\bar{F}}^{s}\%$, it is also useful to plot the results from each simulated sampling survey, in terms of the number of samples that fail F^{s}, in order to depict the possible variation in sampling results. This has been carried out for the plug flow model at each lead standard (Figure 3.29). The histogram clearly illustrates the variation in sampling results, i.e. the spread in F^{s}, at each lead standard across the $m = 100$ surveys simulated. Note that if *RDT* sampling were completely reproducible the histogram would comprise of one single column at each lead standard.

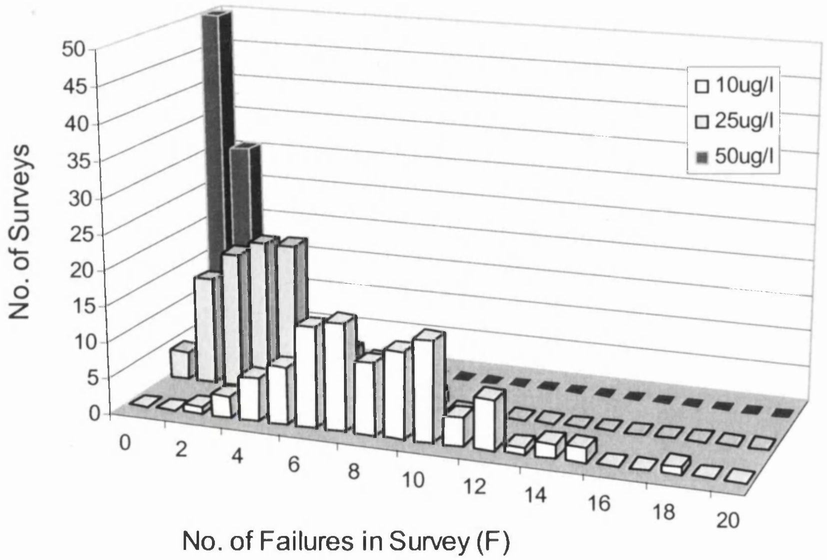


Figure 3.29. Histogram of results from all sampling surveys (Plug).

On closer inspection of Figure 3.29, it is observed that the variation in F^s becomes smaller with increasing lead standard, indeed at the least stringent standard of *50μg/l* F^s is observed to vary between *0* and *3* only.

Similar results are illustrated (Figure 3.30 and Figure 3.31) for the turbulent – exponential and turbulent – diffusion models, though F^s, is noticeably biased towards lower values in the case of the turbulent – exponential model at the *10μg/l* standard.

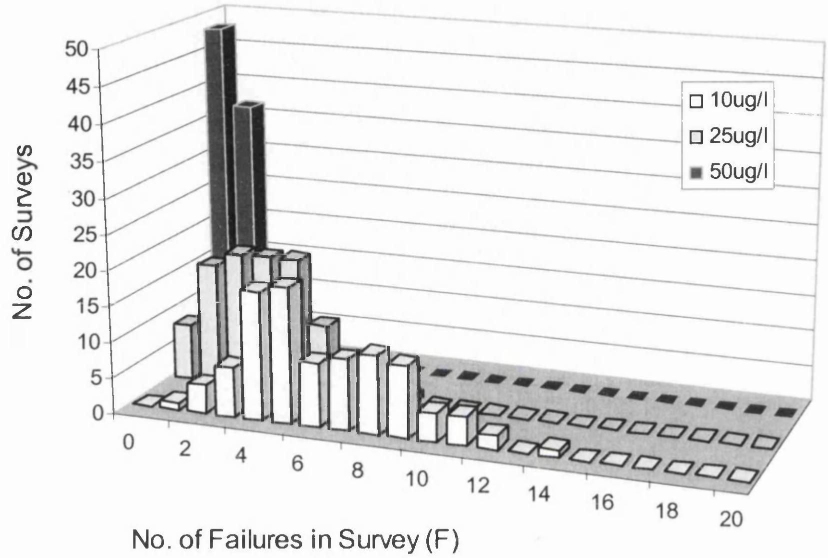


Figure 3.30. Histogram of results from all sampling surveys (Turb-Exp).

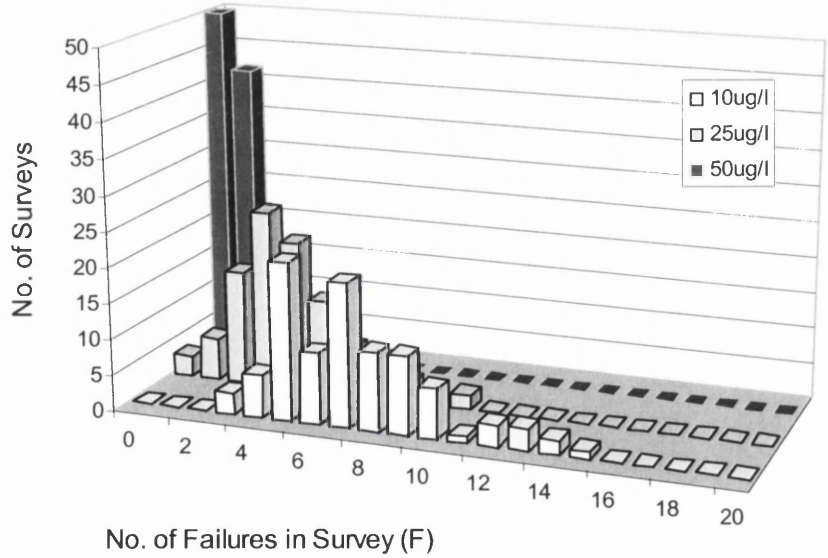


Figure 3.31. Histogram of results from all sampling surveys (Turb-Dif).

3.3.3.4 Confidence limits

From a limited quantity of sample data, it is clear that the true population mean of the *RDT* zonal failure rate cannot be precisely found and must be estimated from the sample mean. However, for the purposes of predicting zonal compliance of a real-world sampling survey, it is of greater benefit to describe the likely range of sampling survey results, in terms of F^s, which could possibly occur, to some statistical level of certainty. This can be achieved by calculating the confidence limits of the *RDT* failure rate, which take the form of upper and lower limits either side of the mean failure rate and are used to describe the confidence interval, i.e. the range of values where the *RDT* failure rate can be expected to lie, to some statistical level of certainty.

In most areas of scientific research, the criterion for statistical significance is conventionally set at the *5%* level (Lowry, R. 1999). This implies that there is only a *5%* chance that an observed *RDT* failure rate will fall outside the confidence interval, this corresponds to a *95%* confidence interval. The *95%* confidence interval of the *RDT* failure rate is defined as:

$$\hat{F}^s\% \pm \left(1.96 \times \hat{\sigma}^s\%\right) \qquad \text{Eqn. 3.10}$$

The upper and lower confidence limits for the *RDT* failure rate that have been computed from the simulation of $m = 100$ surveys are illustrated for the plug flow model (Table 3.3). This illustrates the huge range in sampling survey results that can be expected to occur, particularly at the *10μg/l* standard. Thus, for this standard, observing real-world zonal compliance of *26%* and *5%* for two separate sampling surveys of the same zone is deemed statistically insignificant and is attributable to chance. Consequently, the employment of *RDT* sampling using a relatively small sample size is highly questionable in terms of reproducibility and representing zonal compliance with lead standards in accordance with the new directive to any degree of accuracy. Similar confidence limits are obtained when the turbulent – exponential and turbulent – diffusion models are used.

Table 3.3. Confidence Intervals for *RDT* failure rate (%) from Plug flow model.

	10 μg/l	*25 μg/l*	*50 μg/l*
Mean	15.56	6.35	1.42
Lower Confidence Limit	4.4	0.0	0.0
Upper Confidence Limit	26.7	13.9	4.8

3.3.4 Graphic representation

As previously discussed, the primary output obtained from the simulation of exact assessment is the zonal failure rate for each lead standard, i.e. the percentage of houses where the *DAC* exceeds lead standards of *10μg/l*, *25μg/l*, and *50μg/l*. However, this summary data provides no information regarding the temporal variation of lead emissions that occur across the water supply zone during the simulated day. Such detailed information will allow the water engineer to determine the times during that day when peak lead emissions are observed across the zone as a whole. This will also enable the water supply zone to be assessed in terms of lead emissions at any one point during the simulated day, which may be carried out on pre and post treatment results to observe the effects of corrective treatment.

In order to observe such data instantly, it is necessary to generate a graphical representation of the zone in terms of the varying lead emissions at each property during the simulated day. This has been achieved by representing the zone as an array of N x N coloured pixels, where the size of the simulated zone is N^2. Thus, a zone of *10,000* houses is represented by an array of *100* x *100* colour pixels, each pixel representing a house from the simulated zone. For every point in time during the simulated day, the colour of the pixel is determined by the instantaneous lead emissions computed for the related house. A simple colour coding system is used:

Table 3.4. Colour coding of pixels.

Colour	Instantaneous lead emissions (μg/l)
Green	0 - 10
Yellow	10 - 25
Red	25 - 50
Grey	> 50

This effectively results in an animation that graphically depicts the zonal and temporal variation in lead emissions in terms of colour changes. For practicality the animation runs *60* times faster than the simulated time, i.e. it takes one second of animation to display one minute of results. In order that the observer knows what time during the simulated day the results relate to, the simulated time is displayed within the animations.

Additionally, a bar depicting the proportions of the total zone for each category of lead emissions, i.e. each colour, is displayed within the animation. The provides the observer with a summary for the entire zone in terms of temporal variation of lead emissions only.

Examples of such animations are included with this thesis on the attached CD-ROM and can be played on most modern PCs. These animations show results, in terms of instantaneous lead emissions, obtained from an 'average zone' before and after water treatment at two different time periods during the simulated day. The animations clearly depict the high lead emissions observed for both pre and post treatment at the start of the day during the first-draw after over-night stagnation. However, as the first-draw transpires, the animations reveal the impact of water treatment on lead emissions very clearly.

For obvious reasons these animations cannot be included in the text of this thesis; consequently, for illustrative purposes, several 'snapshots' of the animations are included (Figure 3.32 - Figure 3.34).

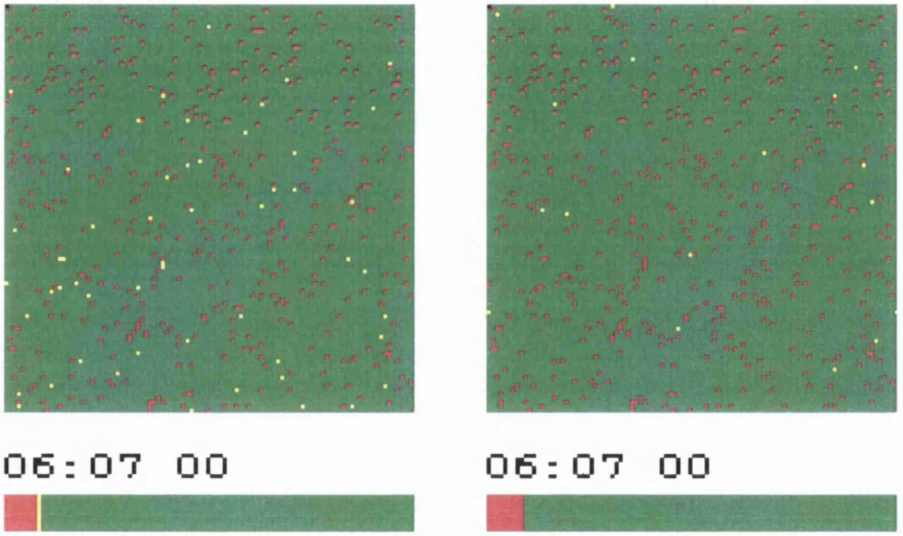


Figure 3.32. Start of first-draw (a) Pre-treatment. (b) Post-treatment.

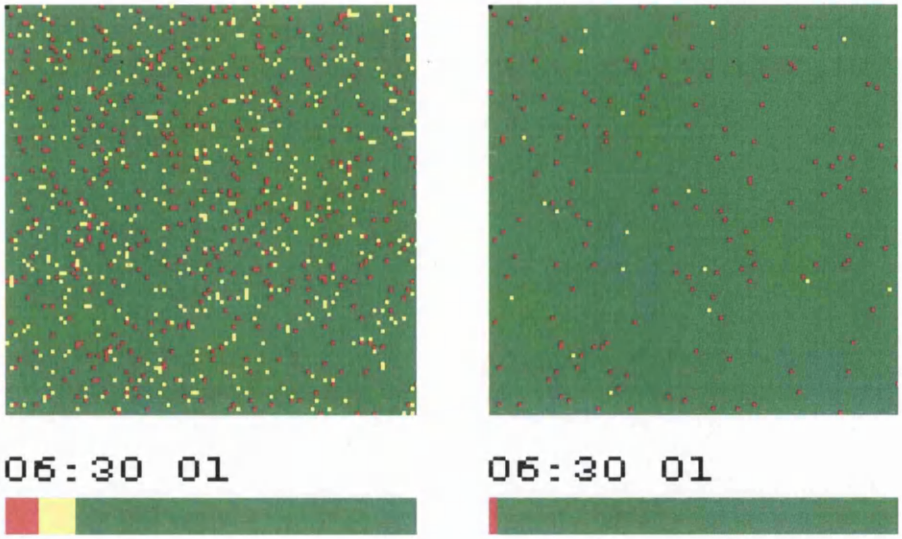


Figure 3.33. End of first-draw (a) Pre-treatment. (b) Post-treatment.

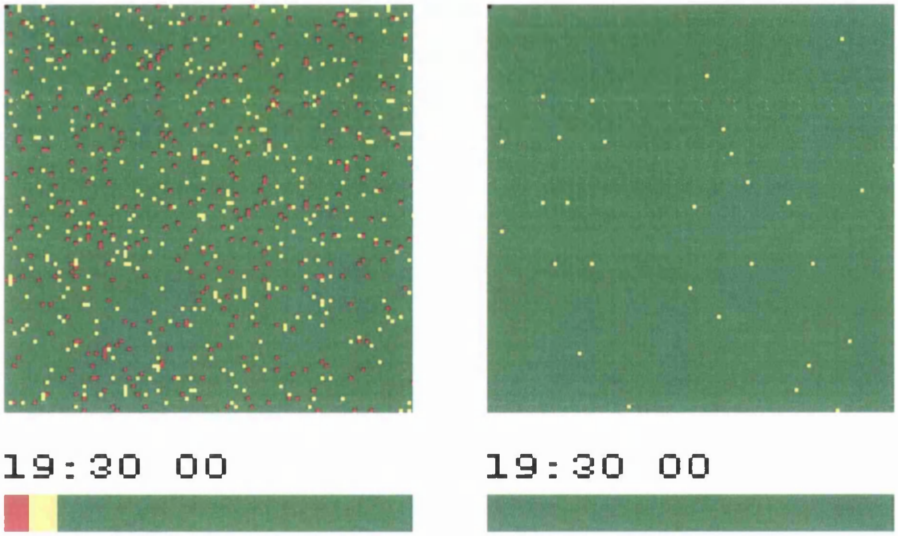


Figure 3.34. Evening (a) Pre-treatment. (b) Post-treatment.

3.4 Sensitivity analyses

3.4.1 Effect of input parameters on exact assessment

In order to understand the general issues that relate to plumbosolvency control on a zonal scale, it is necessary to investigate the influence of zonal factors on compliance, in terms of both exact assessment and RDT sampling. 'Exact' assessment is the most comprehensive method of determining zonal compliance in accordance with the new directive and involves the characterisation of all lead emissions occurring across a zone during one simulated day. The primary output obtained from the simulation of exact assessment is the zonal failure rate for each lead standard, i.e. the percentage of houses where the *DAC* exceeds lead standards of *10µg/l*, *25µg/l*, and *50µg/l*.

The parameters that affect household lead emissions, in terms of *DAC*, include the geometry of the pipework, the water usage and the plumbosolvency of the water, as previously discussed (Chapter 2.4.2). Consequently, it is logical to assume that changes in the distribution used to describe the zonal variation of these household parameters will effect zonal compliance based on exact assessment and therefore require investigation. Additionally, the influence of zonally static parameters, i.e. parameters that are uniformly applied across the simulated zone, must also be investigated. Thus, the following parameters will be investigated, in terms of their influence on zonal compliance based on exact assessment:

- Zonally varying parameters (defined by a distribution)
    - Length of lead pipework
    - Length of copper pipework
    - Total daily volume of water used

- Zonally static parameters (defined by a single value)
    - Plumbosolvency
    - Diameter of pipework

- General properties of the zone
    - Size of zone
    - Proportion of houses that have lead pipework

The influence of each parameter on compliance assessment can be examined simply by altering one parameter at a time, over a suitable range. The remaining parameters in each case are representative of those that may occur for a typical water supply zone and are characterised by those used to generate the 'average' zone having *2,000 houses*, *40%* of which having lead pipework as previously described (Chapter 3.3.2.1).

The investigation of each zonally varying parameter will involve the generation of a number of zones; each generated using a different distribution to represent the zonal variation of that parameter. The most straightforward method of specifying an adjusted distribution is to simply modify the standard distribution by increasing all the discrete values of that parameter by a constant A, whilst maintaining the corresponding probability of obtaining that discrete value. This effectively results in a new distribution for that parameter having a mean of $\mu + A$, where μ is the mean of the standard distribution. Note that the shape of the distribution remains the same and is merely translated by A along the axis of the value of the parameter.

In most cases, solutions of compliance assessment in terms of the zonal failure rate at lead standards of *10µg/l*, *25µg/l*, and *50µg/l* will be illustrated for the plug flow model only, for simplicity. This is because, in general, solutions from the turbulent – exponential and turbulent – diffusion models are found to follow the same pattern to those obtained from the plug flow model. Differences between solutions from the different models can be explained by considering the effect of the flow and mass transfer models on lead emissions at a single house, as previously discussed (Chapter 3.3.2.1).

3.4.1.1 Zonally varying parameters

3.4.1.1.1 Length of lead pipework

Solutions were obtained from *5* zones; each generated assuming a different distribution of length of lead pipework as follows:

- Zone-0: Standard distribution – *5m*
- Zone-1: Standard distribution, (Figure 3.3)
- Zone-2: Standard distribution + *5m*
- Zone-3: Standard distribution + *10m*
- Zone-4: Standard distribution + *15m*

The resulting effect of length of lead pipework on exact assessment is illustrated (Figure 3.35). This shows that the failure rate at each lead standard increases with lead pipe length, essentially a linear relationship.

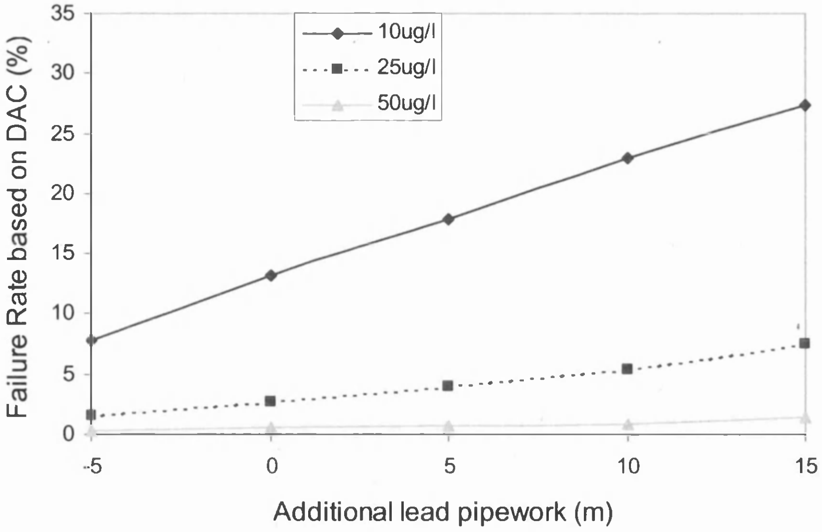


Figure 3.35. Effect of lead pipework length on exact assessment.

These results mirror those obtained for *DAC* at a single house (Chapter 2.4.2.2); a consequence of exact assessment being a function of *DAC* of all houses within the simulated zone. Consequently, the relationship can be explained in the same way, namely the volume of water that is in contact with lead pipework, at any one point in time, increases linearly with length of lead pipework. However, it should be noted that the zonal failure rate, at any lead standard, cannot exceed *40%* since the proportion of houses that have lead pipework within the zone is *40%*.

3.4.1.1.2 Length of copper pipework

The influence of the length of copper pipework was investigated in the same manner as length of lead pipework, however, distributions were adjusted by increments of *2.5m* as opposed to *5m*, reflecting the smaller mean length of copper pipework observed in a standard zone. The resulting effect of length of copper pipework on exact assessment is illustrated (Figure 3.36). This shows that there is no discernable variation in failure rate with length of copper pipework for each lead standard.

Once again, these results mirror those obtained for *DAC* at a single house (Chapter 2.4.2.3), which revealed that length of copper pipework has very little effect on *DAC* for lengths less than *25m*, the maximum normally encountered. Consequently, the insignificant effect of the length of copper pipework on exact assessment can be explained using the principles of conservation of mass, i.e. no lead is generated or destroyed within the copper pipework and hence *DAC* remains unchanged.

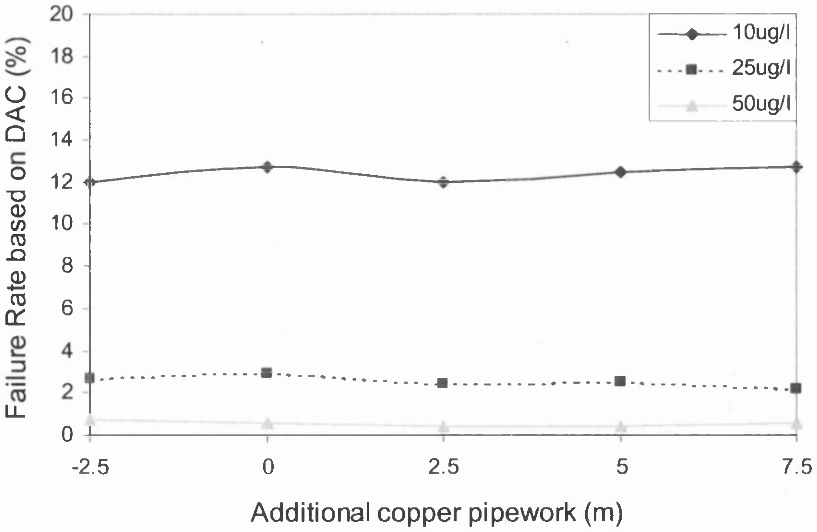


Figure 3.36. Effect of copper pipework length on exact assessment.

Note that despite the insignificant effect of the length of copper pipework, the failure rates are observed to differ slightly with the length of copper pipework, with no apparent relationship. This is a consequence of the random ascription of parameter values during the generation of each zone in this investigation.

3.4.1.1.3 Daily water consumption

The influence of daily water consumption was investigated in the same manner as length of lead pipework; though distributions were adjusted by increments of *25l*. The resulting effect of daily water consumption on exact assessment is illustrated (Figure 3.37). This shows that the failure rate at each lead standard decreases with increasing daily water consumption, the relationship being logarithmic.

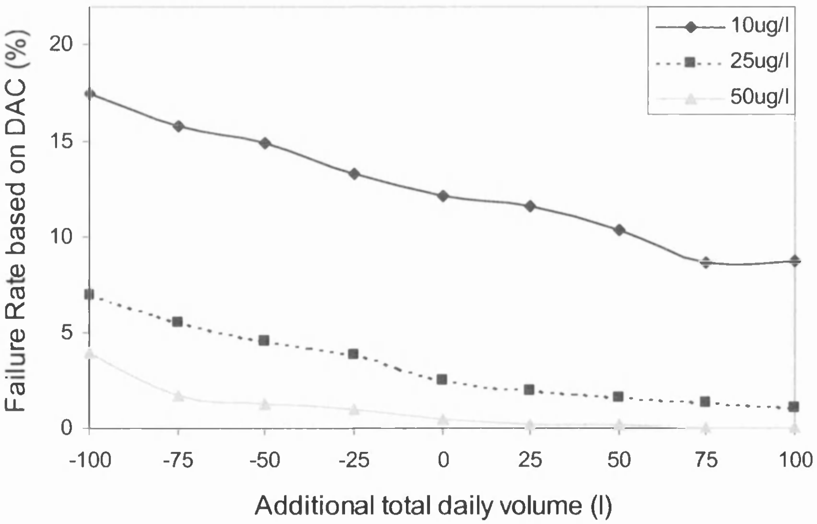


Figure 3.37. Effect of daily water consumption on exact assessment.

As with length of lead pipework, these results mirror those obtained for *DAC* at a single house (Chapter 2.4.2.5), which revealed that *DAC* decreases logarithmically with increasing daily water consumption. Thus, it follows that the relationship can be explained in the same way as previously discussed (Chapter 2.4.2.5).

3.4.1.2 Zonally static parameters

3.4.1.2.1 Pipework diameter

The effect of pipework diameter, uniformly applied across the simulated zone, on exact assessment is illustrated (Figure 3.38). This shows that the failure rate at each lead standard increases with pipework diameter, essentially a linear relationship. Once again, these results mirror those obtained for *DAC* at a single house (Chapter 2.4.2.4); a consequence of exact assessment being a function of *DAC* of all houses within the simulated zone. Thus, the relationship can be explained in the same way as previously discussed (Chapter 2.4.2.4).

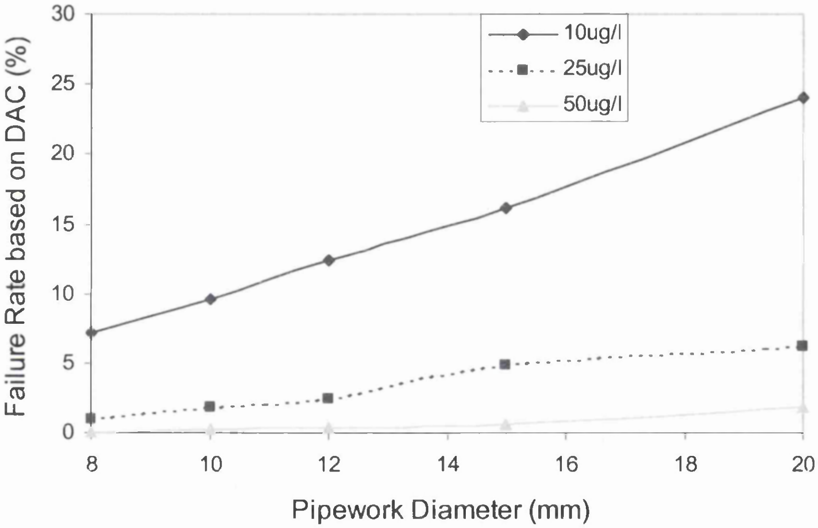


Figure 3.38. Effect of pipework diameter on exact assessment.

3.4.1.2.2 Plumbosolvency

The plumbosolvency of the water is defined by factors *M* and *E* (exponential model) and factors *D* and *E* (diffusion model). An increase in plumbosolvency is characterised by an increase in solubility *E*. However, in the case of the exponential approximation, it is also necessary to increase the initial mass transfer rate, *M* by the same proportion.

The effect of plumbosolvency, uniformly applied across the simulated zone, on exact assessment is illustrated (Figure 3.39). This shows that the failure rate at each lead standard increases with plumbosolvency, essentially a linear relationship. Once again, these results mirror those obtained for *DAC* at a single house (Chapter 2.4.2.1); a consequence of exact assessment being a function of *DAC* of all houses within the simulated zone. Thus, the general relationship can be explained in the same way as previously discussed (Chapter 2.4.2.1).

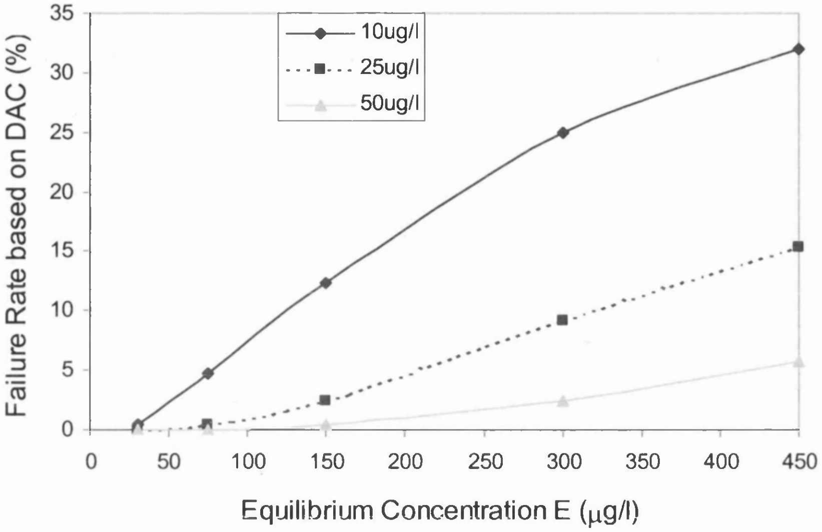


Figure 3.39. Effect of plumbosolvency on exact assessment.

However, it should be noted that a failure rate of zero is observed at each lead standard until the plumbosolvency is set higher than *E = 30μg/l*. Failure rates greater than zero at the *50μg/l* standard are only observed after the plumbosolvency has been increased to at least *E = 150μg/l*. This is because the maximum *DAC* that is likely to be observed for at least *99%* of houses within the zone results from houses having *100m* lead pipework or a daily consumption of just *50l*. Such houses are found to have a *DAC* equal to approximately *30%* of the equilibrium concentration *E*, as previously illustrated (Figure 2.33). A non-zero failure rate at the *50μg/l* standard is only observed when a house in the zone is found to have a combination of very long lead pipework and very low water consumption, resulting in a *DAC* greater than *33%* of the equilibrium concentration *E*, i.e. greater than *50μg/l*.

3.4.1.3 General zonal properties

3.4.1.3.1 Zone size

The effect of zone size on exact assessment is illustrated (Figure 3.40). This shows that the failure rate at each lead standard effectively remains constant with increasing zone size as expected since failure rate is expressed as a percentage of the total zone.

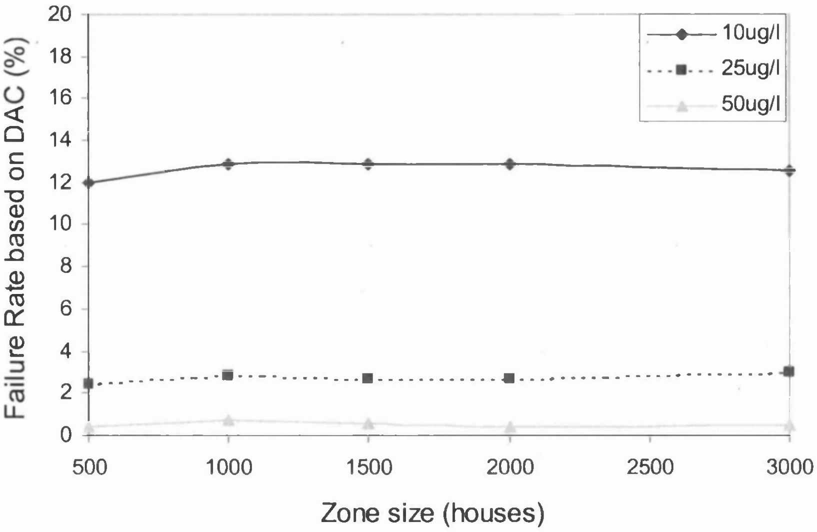


Figure 3.40. Effect of zone size, H_T on exact assessment.

However, note that the failure rates are observed to differ slightly with zone size; this being a consequence of the random ascription of parameter values during the generation of each zone in this investigation.

3.4.1.3.2 Proportion of houses that have lead pipework

The effect of the proportion of houses that have lead pipework on exact assessment is illustrated (Figure 3.41). This shows that, as expected, the failure rate at each lead standard increases with the proportion of houses that have lead pipework, essentially a linear relationship.

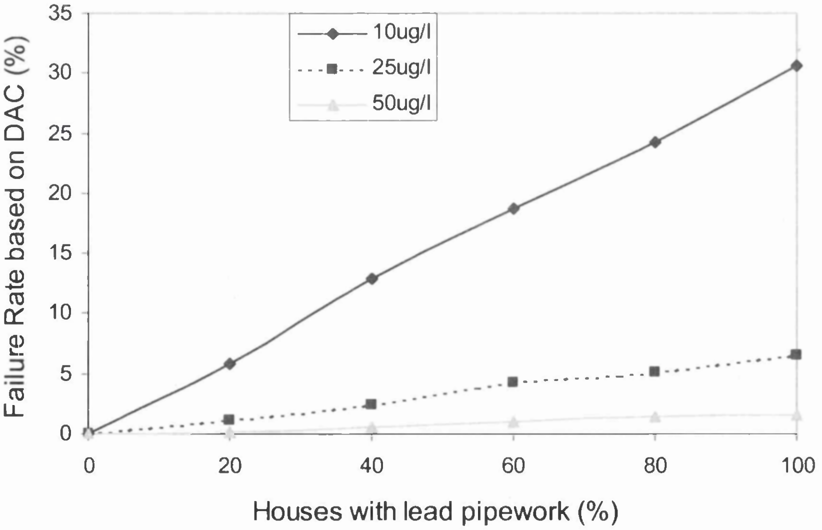


Figure 3.41. Effect of the proportion of houses supplied through lead pipework, *Pb%* on exact assessment.

3.4.2 Effect of input parameters on RDT sampling

The most widely used sampling technique employed by water suppliers in the UK, is Random Day Time (*RDT*) sampling. Consequently, in order to understand the general issues that relate to plumbosolvency control in a way that is representative of real-world compliance assessment, *RDT* sampling simulations will be employed for the investigation of the influence of zonal factors on compliance.

The simulated *RDT* sampling surveys to be carried out will comprises $n = 52$ samples in order to represent a typical *RDT* sampling survey, which is carried out over one year with one sample being taken from the water supply zone each week. However, since *RDT* sampling survey results are never completely reproducible the simulated survey will be repeated $m = 100$ times, in order to be able to understand possible variation. The primary output obtained from the simulation of *RDT* sampling is the zonal failure rate for each lead standard, i.e. the percentage of *RDT* samples where the sample concentration exceeds lead standards of $10\mu g/l$, $25\mu g/l$, and $50\mu g/l$.

Unlike the standard *30MS* (30-Minute Stagnation) test, previously discussed (Chapter 1.1.9.1.2), *RDT* sample collection is carried out with no prior flushing. Consequently, the *RDT* sample concentration is influenced by the water usage at that house up to the point that the sample is taken. Thus, parameters that relate to water usage, such as the pattern of water usage and the daily water consumption, will affect the *RDT* sample concentration and must be investigated.

Other parameters that affect *RDT* sample concentration include the geometry of the pipework and the plumbosolvency of the water. As in the case of exact assessment, it is logical to assume that changes in the distribution used to describe the zonal variation of these household parameters will effect zonal compliance based on *RDT* sampling and therefore require investigation. Additionally, the influence of zonally static parameters, i.e. parameters that are uniformly applied across the simulated zone, must also be investigated. Thus, the following parameters will be investigated, in terms of their influence on zonal compliance based on *RDT* sampling:

- Zonally varying parameters (defined by a distribution)
    - Length of lead pipework
    - Length of copper pipework
    - Total daily volume of water used

- Zonally static parameters (defined by a single value)
    - Plumbosolvency

    - Diameter of pipework

- General properties of the zone
    - Size of zone
    - Proportion of houses that have lead pipework

The influence of each parameter on *RDT* sampling results can be examined simply by altering one parameter at a time, over a suitable range. The remaining parameters in each case are representative of those that may occur for a typical water supply zone and are characterised by those used to generate the 'average' zone having *2,000 houses*, *40%* of which having lead pipework as previously described (Chapter 3.3.2.1). As in the case of exact assessment, the investigation of each zonally varying parameter will involve the generation of a number of zones; each generated using a different distribution to represent the zonal variation of that parameter.

In most cases, solutions of compliance assessment in terms of the zonal failure rate at lead standards of *10µg/l*, *25µg/l*, and *50µg/l* will be illustrated for the plug flow model only, for simplicity. This is because, in general, solutions from the turbulent – exponential and turbulent – diffusion models are found to follow the same pattern to those obtained from the plug flow model. Differences between solutions from the different models can be explained by considering the effect of the flow and mass transfer models on lead emissions at a single house, as previously discussed (Chapter 3.3.3).

3.4.2.1 Zonally varying parameters

3.4.2.1.1 Length of lead pipework

Solutions were obtained from *5* zones; each generated assuming a different distribution of length of lead pipework as previously described (Chapter 3.4.1.1.1). The resulting effect of length of lead pipework on *RDT* sampling results is illustrated (Figure 3.42). This shows that the failure rate at each lead standard increases with lead pipe length, essentially a linear relationship. However, note that the failure rate at the *10µg/l* standard is slightly lower than expected when the additional lead pipework length is set to *–5*. This is because a significantly large proportion of *RDT* sample concentrations are found to be slightly less than *10µg/l* as opposed to slightly greater than *10µg/l*, when the average length of lead pipework is reduced by *5m*.

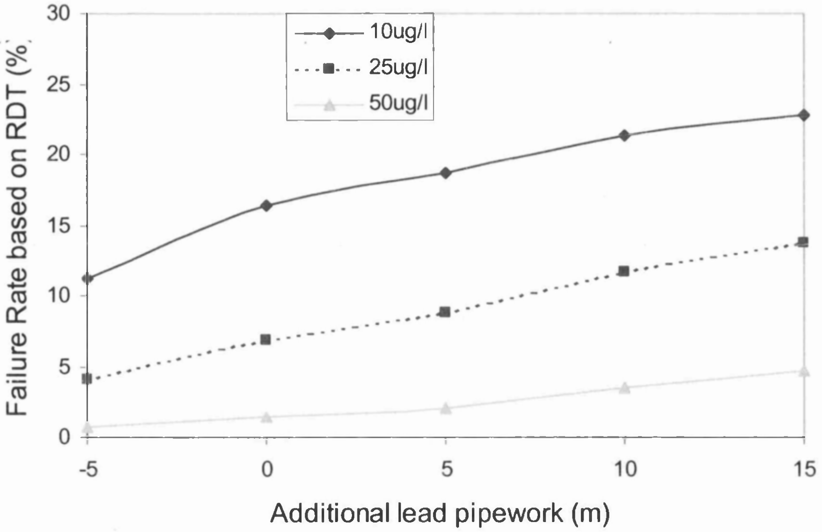


Figure 3.42. Effect of lead pipework length on *RDT* sampling.

Note that these results mirror those obtained for exact assessment, a consequence of *RDT* sampling results being a influenced by the lead emissions occurring throughout the simulated day of all houses within the simulated zone. Once again, note that the zonal failure rate, at any lead standard, cannot exceed *40%* since the proportion of houses that have lead pipework within the zone is *40%*.

3.4.2.1.2 Length of copper pipework

The effect of length of copper pipework on *RDT* sampling results is illustrated (Figure 3.43). This shows that, as opposed to exact assessment, *RDT* sampling results are noticeably affected by the length of copper pipework, particularly at the *10µg/l* standard.

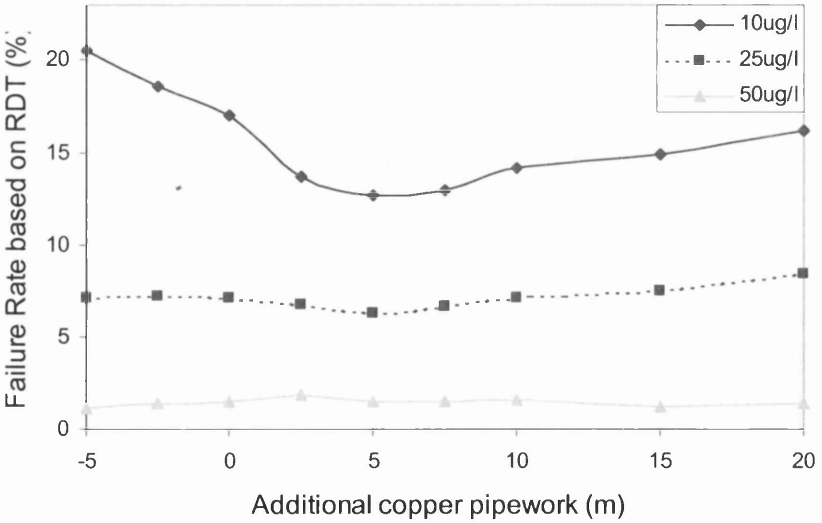


Figure 3.43. Effect of copper pipework length on *RDT* sampling.

The initial decrease in failure rates with increasing lengths of copper pipework is a result of the dilution effect, which is also observed in the *30MS* test. The dilution effect can be explained by considering that the *1-litre RDT* sample, taken at the tap, will be comprised of water that has stagnated in the copper pipework, and water that has stagnated in the lead pipework if the length of copper pipework is shorter than *10m*.

When the length of copper pipework is relatively short, i.e. *10m* or less, it is likely that the total pipework will effectively be flushed of water that contains lead during a typical flow period. Consequently, since the *RDT* sample will likely be taken during a stagnation period, it follows that, at the time of sample collection, the concentration of lead in the lead pipework will be significantly greater than the concentration of lead in the lead copper. Thus, *RDT* sample concentration decreases with length of copper pipework since the proportion of water that has stagnated in the copper pipework is proportional to the length of copper pipework.

However, it is observed that as the length of copper pipework is further increased, the failure rates at the *10µg/l* and *25µg/l* standards slowly increase. This is in contrast to the *30MS* test, where it is observed that a copper pipework length greater than *10m* results in a *30MS* sample concentration of zero. Once again, the difference between *30MS* and *RDT* test results can be explained by the water usage, i.e. *RDT* sample collection is carried out with no prior flushing and is thus influenced by previous water usage at that house. In cases of long copper pipework, particularly at houses having low daily water consumption, the duration of the flow period is no longer adequate to completely flush the lead from all of the pipework at that house. Consequently, water stagnating within a proportion of the copper pipework will have a high lead concentration, thus elevating *RDT* sample concentration.

3.4.2.1.3 Daily water consumption

The effect of daily water consumption on *RDT* sampling results is illustrated (Figure 3.44). This shows that the failure rate at each lead standard decreases with increasing daily water consumption, the relationship generally being observed as logarithmic.

These results essentially mirror those obtained for exact assessment. This is because as water consumption decreases, the average flow duration must also decrease assuming a fixed inter-use time. Consequently, water being supplied to the house will have stood in the pipework for increasing lengths of time, producing the compound effect previously discussed (Chapter 2.3.3), thus elevating *RDT* sample concentration.

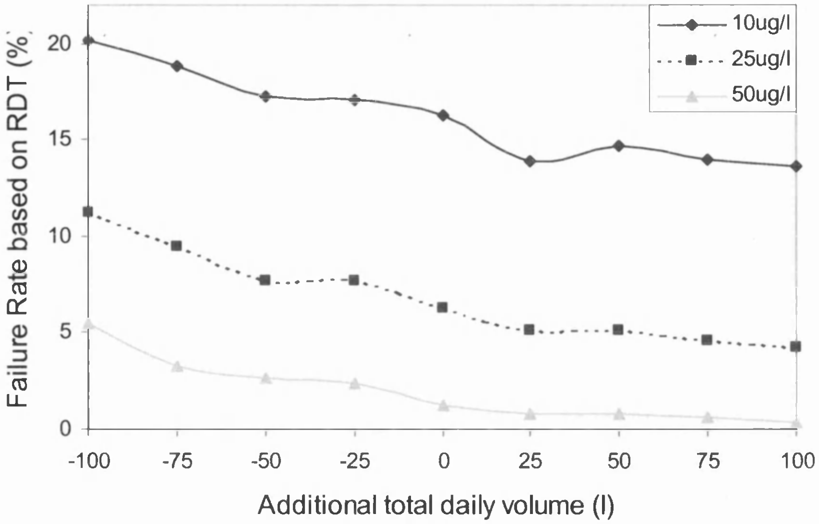


Figure 3.44. Effect of daily water consumption on *RDT* sampling.

3.4.2.2 Zonally static parameters

3.4.2.2.1 Pipework diameter

The effect of pipework diameter, uniformly applied across the simulated zone, on *RDT* sampling results is illustrated (Figure 3.45). This shows that failure rates at the *10µg/l* and *25µg/l* standards increase with pipework diameter while failure rates at the *10µg/l* standard initially decrease and then increase for pipework diameters greater than *12mm*.

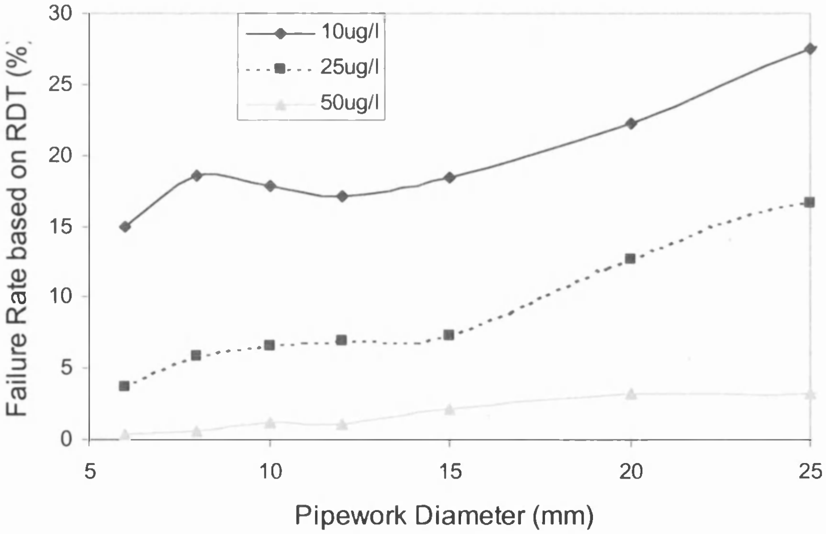


Figure 3.45. Effect of pipework diameter on *RDT* sampling.

This result is in contrast to that obtained for the *30MS* test where it was observed that *30MS* sample concentration decreased logarithmically with increasing pipework diameter. Once again, the difference between *30MS* and *RDT* test results can be explained by the water usage, i.e. *RDT* sample collection is carried out with no prior flushing and is thus influenced by previous water usage at that house. It is observed that the result for *RDT* sampling (Figure 3.45) has more in common with results for *DAC* (Figure 2.35) than for *30MS* (Figure 2.43).

In cases of large pipework diameter, particularly at houses having low daily water consumption, the duration of the flow period is no longer adequate to completely flush the lead from all of the pipework at that house. Consequently, water stagnating within a proportion of the copper pipework will have a high lead concentration, thus elevating *RDT* sample concentration.

However, at a pipework diameter of *8mm*, the failure rate at the *10µg/l* standard becomes slightly elevated. This is because the volume of water contained within the copper pipework reduces with pipework diameter, which results in the *1-litre RDT* sample being comprised of a smaller proportion of water that has been standing in the copper pipework. Since the concentration of lead is likely to be lower in the water contained within the copper pipework, it follows that the *RDT* sample concentration will become slightly elevated; assuming the total length of pipework is not short. However, as pipework length or pipework diameter reduces, *RDT* sample concentration will reduce, as the total volume of the pipework becomes significantly less than *1 litre*, and the *RDT* sample becomes comprised of an increasing proportion of fresh water from the water main.

3.4.2.2.2 Plumbosolvency

The effect of plumbosolvency, uniformly applied across the simulated zone, on *RDT* sampling results is illustrated (Figure 3.46).

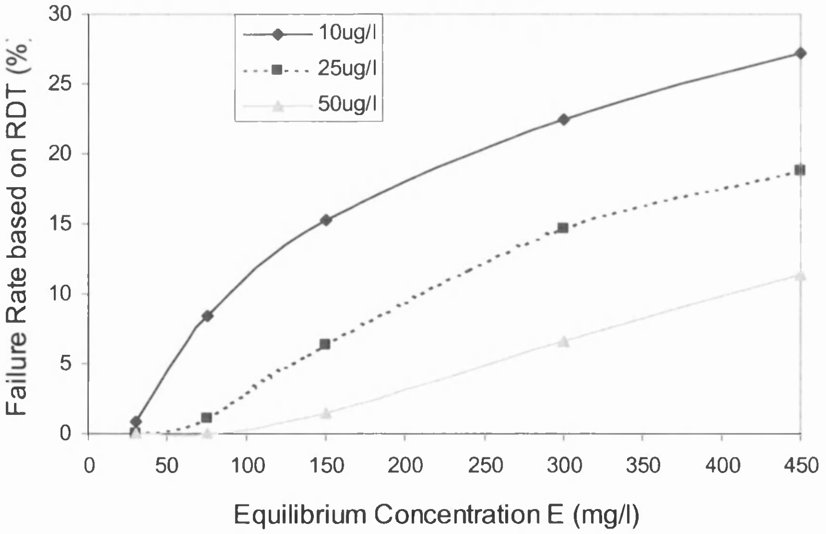


Figure 3.46. Effect of plumbosolvency on *RDT* sampling.

Figure 3.46 illustrates that the failure rate at each lead standard increases with plumbosolvency. The relationship is logarithmic with a sharp initial increase in failure rate with increasing plumbosolvency at the *10μg/l* standard. It should be noted that the relationship is not linear because there will always be occasions when *RDT* samples are taken at the very start of a stagnation period, a result of the sample collection time being randomly chosen. The resulting *RDT* sample concentration on such occasions will always be low, no matter how high the plumbosolvency.

Failure rates greater than zero at the *50μg/l* standard are only observed after the plumbosolvency has been increased to at least *E = 100μg/l* as opposed to *E = 150μg/l* for exact assessment. This is because the maximum *RDT* sample concentrations observed are likely to be greater than the maximum *DAC*s observed within a zone. This is because the maximum *RDT* sample concentrations reflect the maximum instantaneous lead emissions that occur within the zone only, while *DAC*, by definition of being an average, must also incorporate the lower emissions observed at a house.

3.4.2.3 General zonal properties

3.4.2.3.1 Zone size

The effect of zone size on *RDT* sampling results is illustrated (Figure 3.47). This shows that the failure rate at each lead standard effectively remains constant with increasing zone size as expected since failure rate is expressed as a percentage of the total zone.

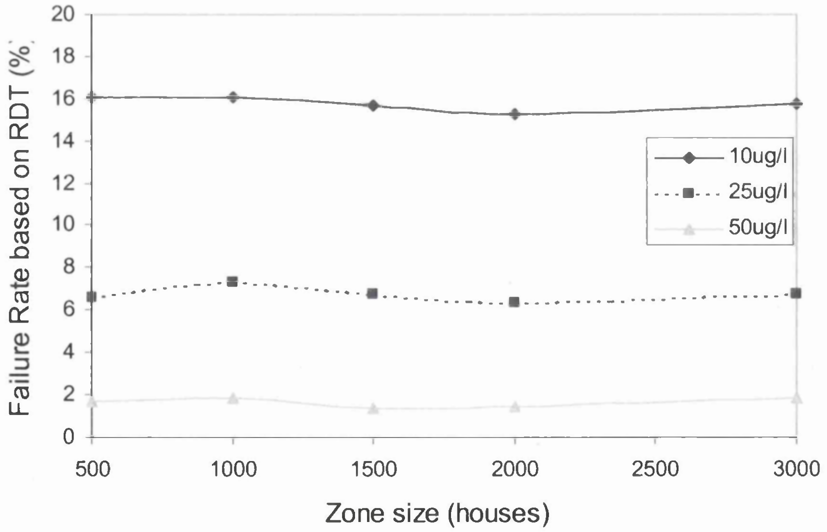


Figure 3.47. Effect of zone size, H_T on *RDT* sampling.

However, note that the failure rates are observed to differ slightly with zone size; this being a consequence of the random ascription of parameter values during the generation of each zone in this investigation.

3.4.2.3.2 Proportion of houses that have lead pipework

The effect of the proportion of houses that have lead pipework on *RDT* sampling results is illustrated (Figure 3.48). This shows that, as expected, the failure rate at each lead standard increases with the proportion of houses that have lead pipework, essentially a linear relationship.

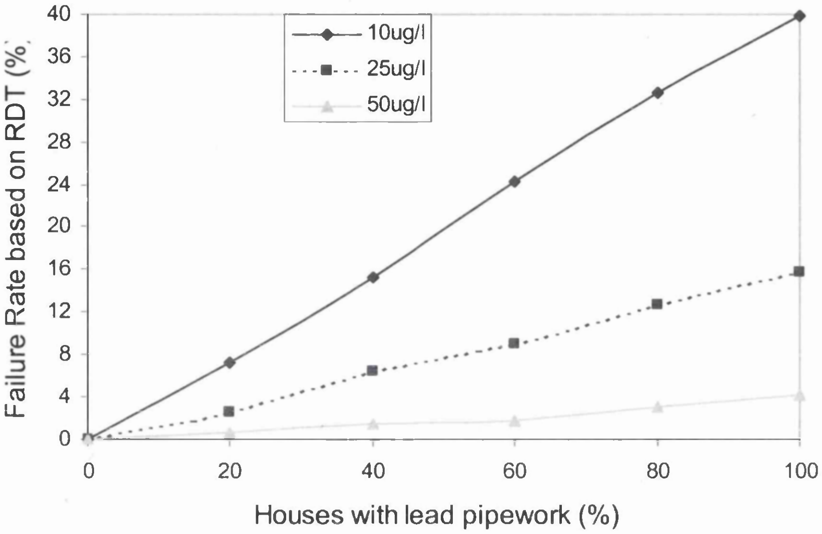


Figure 3.48. Effect of the proportion of houses supplied through lead pipework, *Pb%* on *RDT* sampling.

3.4.3 Effect of discretisation

In order to model spatial and temporal variations in concentration at a single house, it has been necessary to discretised the domain, i.e. the pipework, and also discretise the time for which a stagnation or flow period takes place, as previously described (Chapter 2.2.1.3). The resolution of the temporal discretisation was chosen as $\Delta t = 1\ sec$, for simplicity. For the standard assumptions of $Q = 0.1 l/s$ and $r_o = 6mm$, this timestep resulted in a spatial resolution of $\Delta x = 0.88m$, $1.77m$ and $1.08m$ for plug-flow, laminar flow and turbulent flow, respectively. The application of this chosen discretisation was justified for the computation of lead emissions at a single house.

In order to justify the application of this chosen discretisation for the computation of zonal compliance, it is necessary to investigate the influence of discretisation on both exact assessment and RDT sampling. Investigations are carried using the 'average' zone having *2,000 houses*, *40%* of which having lead pipework as previously described (Chapter 3.3.2.1). As with investigation of the effect of input parameters, solutions of compliance assessment in terms of the zonal failure rate at lead standards of $10\mu g/l$, *25μg/l*, and *50μg/l* will be illustrated for the plug flow model only, for simplicity. Consequently, the effect of discretisation in the axial direction will be investigated only.

3.4.3.1 Exact assessment

The effect of pipe discretisation on exact assessment is illustrated (Figure 3.49).

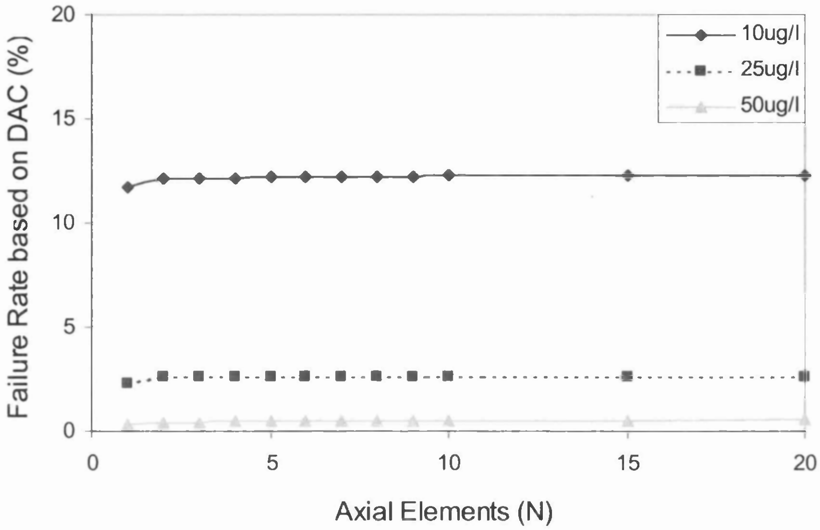


Figure 3.49. Effect of discretisation on exact assessment.

Clearly, axial discretisation has very little effect on exact assessment. This result mirrors that obtained for *DAC* at a single house (Chapter 2.4.4.2); a consequence of exact assessment being a function of *DAC* of all houses within the simulated zone. Axial discretisation has little effect because *DAC* is computed as an aggregate value from all lead emissions occurring during the simulated day. Since conservation of mass is imposed within the model for a single house, it follows that average concentration, expressed as *DAC* for a simulated day, must remain constant.

3.4.3.2 RDT sampling

The effect of pipe discretisation on *RDT* sampling results is illustrated (Figure 3.50). Axial discretisation has a significant effect on *RDT* sampling results, particularly when the discretisation is course. This is because the *RDT* sample concentration is determined in only *10 seconds* of flow and is thus sensitive to instantaneous concentration variations over space and time.

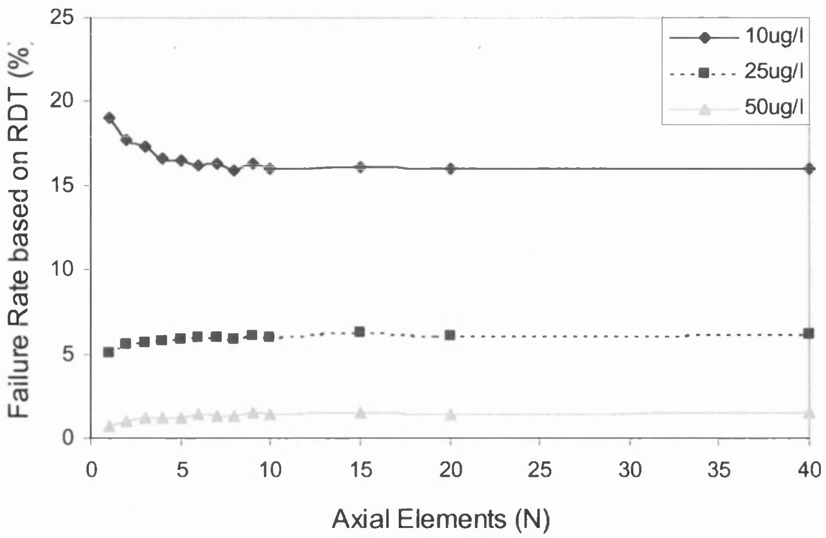


Figure 3.50. Effect of discretisation on RDT sampling.

As the amount of discretisation is increased, the failure rates at the more stringent lead standard of *10μg/l* decrease, whilst the failure rates at the less stringent lead standards of *25μg/l* and *50μg/l* increase (Figure 3.50). When higher levels of discretisation are used, instantaneous responses are portrayed more accurately since the greater spatial resolution can capture the sharp spikes in lead concentration within the pipework. In the extreme case where only one element is to be used to represent the entire lead pipework, the sharp peaks in concentration cannot be captured since the lead concentration is effectively computed as an average value over the entire length of the pipework. This causes an artificial smoothing of the concentration being output, which, in the case of events such as sampling, has a marked effect.

3.5 Shared communication pipes

3.5.1 Introduction

In most water supply zones in the U.K. the housing is almost exclusively detached, semi-detached or terraced. In these cases the properties are supplied with drinking water from the water main via a single communication pipe as depicted in Figure 1.5. However, water supply zones in cities or at the centre of large towns are likely to contain a significant proportion of properties in the form of high-rise flats or apartment blocks. Such properties will usually be supplied with drinking water via a SCP (Shared Communication Pipe) as depicted in Figure 1.8. Additionally, it has been found that the housing in some European cities is predominantly connected through SCPs [61], particularly where houses are terraced and adjacent to the road, i.e. have no front garden.

Water supply zones having significant proportions of houses connected through SCPs cannot be modelled in the same way as standard water supply zones, i.e. zones having no SCPs. This is because the water usage of one house can effect the lead emissions at another house if both houses share the same lead communication pipe, as previously discussed (Chapter 1.2.4.2).

Consequently, in order to predict zonal compliance and investigate the effects of treatment in zones having SCPs, it is necessary to model the structure of such a water supply zone. This will enable the effect of SCPs on lead emissions to be quantified and allow for a more accurate description of a real-world water supply zone.

3.5.2 Mathematical description

A general description of a water supply zone with SCPs can be developed in much the same way as a standard zone, previously discussed (Chapter 3.1). However, in addition to data that describes the properties of each house in the zone, it is necessary to include data that describes the properties of each SCP in the zone. Furthermore, it is necessary to include data that describes the configuration of the zone in terms of which houses connect to which SCPs.

Consequently, the data required to describe a zone with SCPs can essentially be structured into a list of houses and the household properties at each house as well as a list of communication pipes and their properties. This zonal data can be stored in an array as:

$$Zone = Houses[Address(i), Household\_Properties(i)] + SCP$$
$$[Address(k), Comm\_Pipe\_Properties(k)]$$

Eqn. 3.11

$$for\ i = 1,\ H_T$$

$$for\ k = (H_T+1),\ (H_T+1)+C_T$$

where H_T is the total number of houses in the zone and C_T is the total number of SCPs in the zone. Note that *Address* is simply a reference number for a house or SCP. In this manner, all the components in the zone are stored in one single list, with the first H_T entries referring to houses and the last C_T entries referring to SCPs.

In order to describe how the houses and SCPs are connected within the zone, it is necessary to specify the address of the SCP to which each house is connected. The 'SCP address' assigned to house *i, Parent(i),* is stored within the household properties data.

In the simplest case, all SCPs within a zone are connected directly to the water main. However, for flexibility, it is necessary to have the facility to describe zones having more complex configurations, e.g. where a number of SCPs connect to a larger SCP as opposed to the water main. This situation may occur in a large residential building.

It follows that in the case of more complex configurations it will be necessary to specify the address of the larger SCP to which each SCP is connected. The 'larger SCP address' assigned to communication pipe *k, Parent(k),* is stored within the communication pipe properties data.

Where a house or a SCP connects directly to the water main, the address of the Parent pipe is simply stored as zero. This facilitates the description of a zone having houses that are directly connected to the water main, as well as having SCPs in varying levels of complexity.

3.5.3 Communication pipe properties

SCPs are treated simply as a length of lead pipe, although in reality they may also be made from non-lead materials, such as copper. The justification for this is that houses sharing a non-lead communication pipe can be simply treated as being independent and connected directly to the water main, since lead emissions will not be effected.

As with household pipework, it is assumed, for simplicity, that the SCP is perfectly straight; although in reality there may be a number of bends in the pipework. The justification for this is to facilitate the modelling of otherwise highly complex fluid and mass transfer processes whilst keeping enough detail to allow for an accurate representation of the situation.

It is clearly not logistically practical to quantify the properties of every single SCP in a real-world water supply zone. Consequently, it is necessary to be able to model a real-world zone using the limited data obtained through surveys and investigations. This can be achieved by applying the methodology used previously to represent the variation in household parameters across a zone. Thus, the length of SCPs is defined as a discrete distribution, which can be further calibrated to real-world data where available.

In the same manner as household lead length; it is logical to assume that zonal variation of length of SCP follows an asymmetric distribution, biased towards shorter lengths. This skewed distribution is characteristic of a Log-Normal distribution, having a mean of approximately *5m*, after which the proportion of houses having longer lead pipework rapidly decreases (Figure 3.51).

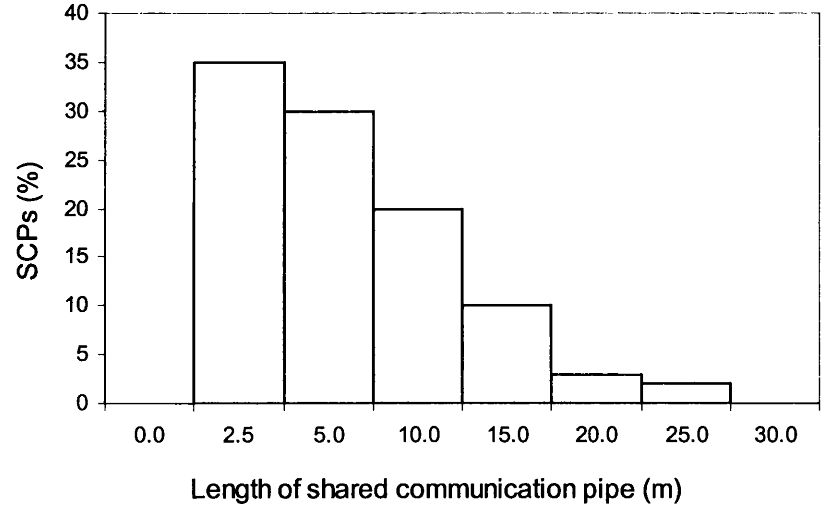


Figure 3.51. Distribution of shared communication pipe length.

Houses supplied through SCPs are likely to have shorter household (non-shared) pipework than houses that are not supplied through SCPs. This is because the SCP effectively replaces a portion of the household pipework. Consequently, it is necessary to specify a separate distribution of household lead pipework length for houses having a SCP. This distribution (Figure 3.52) is very similar in form to that for houses that are not supplied through SCPs (Figure 3.3), though it is further skewed towards shorter lengths of lead pipework.

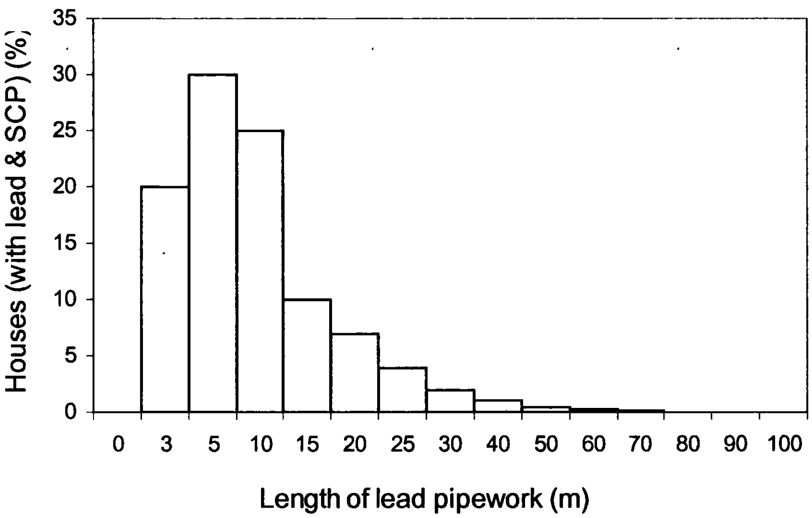


Figure 3.52. Distribution of lead pipework length for houses having a SCP.

The internal diameter of household pipework is generally found to be *12mm* in the U.K. However, pipework diameter of SCP can often be greater than *12mm*, particularly if the SCP supplies three or more houses or flats. Consequently, SCP diameter must be specified as a weighted range, which can be calibrated further where survey data is available.

As with household parameters, SCP length and diameter are randomly ascribed through application of the Monte Carlo procedure previously discussed (Chapter 3.2.2).

3.5.4 Connectivity in a branched system

The typical physical configuration of the SCP and the connecting household pipework is characterised by Figure 1.8. However, for simplicity, this basic configuration will be modelled as a straight SCP connecting directly, at the same location, to the household pipework of all the houses to which it supplies water. In order to describe the method by which a SCP zone is modelled, both in terms of configuration and lead emissions, it is necessary to introduce a simple naming convention. This is particularly important in the case of more complex zones, where it is necessary to distinguish between SCPs that connect to houses and larger SCPs that connect the smaller SCPs to the water main.

An arbitrary SCP zone can be thought of as a hierarchical structure, working from the single water main, through several SCPs to the many houses within the zone. Figure 3.53 illustrates an order-3 zone, i.e. the water flows through a maximum of 3 different pipes (all household pipework is treated as one single pipe) between the water main and the tap. In contrast, a standard zone, i.e. a zone without SCPs, is an order-1 zone.

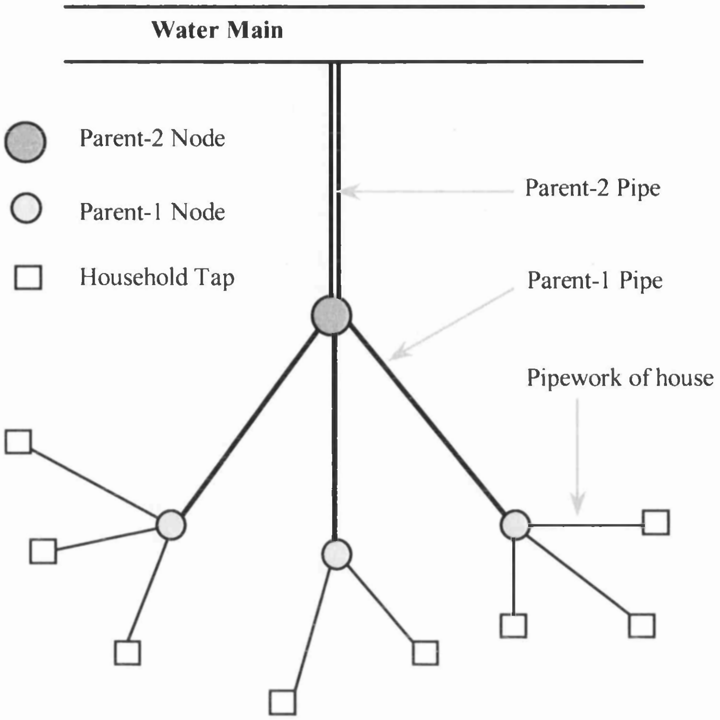


Figure 3.53. Connectivity within part of a zone having SCPs.

The naming convention is summarised as follows:

- Parent-1 Pipe: A SCP that connects directly to household pipework, either from another SCP or from the water main.
- Parent-1 Node: The single point where the Parent-1 Pipe connects to the pipework of all the houses to which it supplies water.
- Parent-2 Pipe: A SCP that connects a Parent-1 Pipe to the water main.
- Parent-2 Node: The single point where the Parent-2 Pipe connects to the Parent-1 Pipe.

Clearly, for more complex networks still, the convention can be extended to include Parent-3 Pipe and Parent-3 Nodes etc.

It is clearly not logistically practical to manually specify the exact configuration of a SCP zone in terms of how every single house and SCP are connected. Consequently, a description of the configuration must be created automatically from more general data relating to the connections within the zone. General data required for creating a complete description of all connections within an order-2 zone include:

- Percentage of houses that are directly connected to the water main (without a SCP).
    - Percentage of these that have lead pipework

- Percentage of houses that are connected to a SCP.
  - Distribution of the number of houses connected to a single SCP (e.g. 25% of houses share with one other house, 50% share with two other houses, 25% share with 3 other houses).
    - Percentage of these that have lead pipework

From this data, the houses within a SCP zone are split up accordingly and assigned SCP addresses where appropriate. As in the case of a standard (non SCP) zone, household parameters and SCP parameters are randomly ascribed through application of the Monte Carlo procedure previously discussed (Chapter 3.2.2). Hence the complete configuration of a real-world water supply zone that has shared communication pipes can be modelled and stored.

3.5.5 Simulation of compliance assessment

In order to predict zonal compliance with the lead standards or investigate the likely effects of corrective water treatment in a SCP zone, it is necessary to evaluate lead emissions across the stored SCP zone in accordance with the method of compliance assessment. The primary methods of assessment that can be simulated are 'exact' assessment and RDT sampling, previously discussed (Chapter 3.2.4).

3.5.5.1 Exact assessment of compliance

For a standard (non SCP) zone, exact assessment of zonal compliance is simulated by applying the model for a single house to each address within the stored description of the zone that has lead pipework. However, this simple approach can no longer be applied where a house is connected to a SCP. This is because lead emissions observed at houses with SCPs are a function of both household parameters and lead emissions produced from the SCP that they connect to. This implies that the input concentration of lead into the pipework of houses with SCPs is non-zero, as opposed to zero for houses connecting directly to the water main.

It should be noted that the SCP connecting a house to the water main cannot simply be treated as part of the household pipework because the concentration of lead within is influenced by the water usage of the other houses that connect to it. Additionally, if more than one house draws water at the same time during the day, then the flow rate within the SCP must increase accordingly. Consequently, it is necessary to consider the water usage of all houses that connect to a SCP concurrently.

By effectively combining the water usage pattern of all houses that connect to a SCP, a new water usage pattern is generated for the SCP itself. Since the flow frequency and flow duration will vary from house to house, it is necessary to generate a water usage pattern for the SCP that has a resolution of one timestep, i.e. *1 sec.* Furthermore the water usage pattern for the SCP must also specify the flow rate that will occur at each second throughout the day, since this will vary depending on the number of houses drawing water at the same time.

Assuming the SCP is directly connected to the water main, the concentration of lead being output at the end of the SCP (the Parent-1 Node) is calculated using the same general procedure for simulating lead emissions at a single house, previously described (Chapter 2.2.5). This concentration is stored for every second during the simulated day and is then used as the input concentration for each house the SCP connects to. Thus, daily lead emissions at SCP houses are computed after the daily lead emissions in the SCP have been evaluated. Consequently, zonal assessment for a SCP zone consists of a pre-processing stage for each SCP that connects to the water main, followed by the standard procedure of assessing lead emissions at each house, though using the input concentration data obtained from the pre-processing stage as opposed to zero. The exact assessment simulation of an order-2 SCP zone can be characterised by the flow diagram illustrated (Figure 3.54).

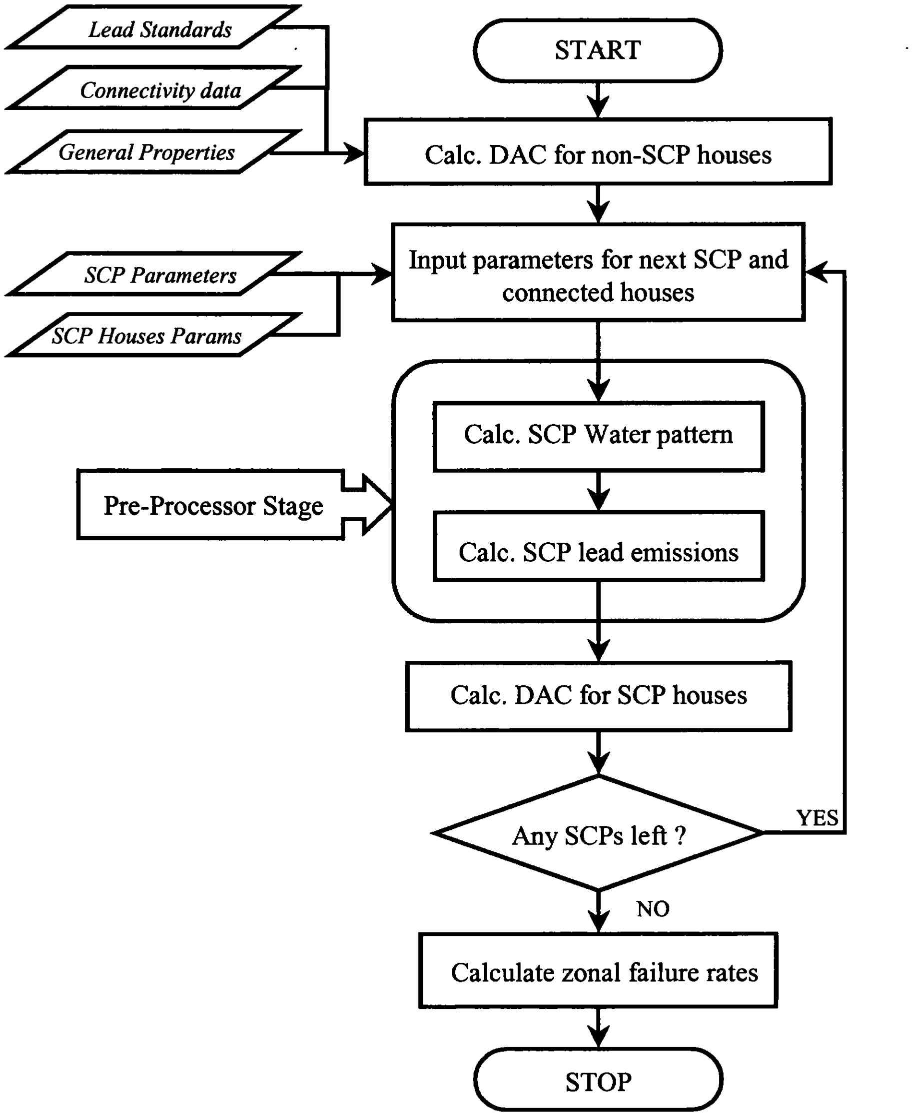


Figure 3.54. Simulation of exact compliance assessment for a SCP zone.

This process of compliance assessment can be extended to more complex SCP zone configurations, e.g. an order-3 SCP zone. In such case, it is necessary to calculate the water pattern of each Parent-2 Pipe by first calculating the water patterns of the connecting Parent-1 Pipes. The lead emissions at the end of the Parent-2 Pipe (the Parent-2 Node) are then calculated and used as the input concentration to the Parent-1 Pipe. A general algorithm describing the process of compliance assessment for an order-N SCP zone is as follows:

1. Calculate DAC for non-SCP houses.
2. Isolate an independent section of the SCP zone that has one Parent-N pipe connecting to the water main.
    a. Pre-process the independent section of the SCP zone (procedure detailed below).

   b. Calculate DAC for all SCP houses in independent section of SCP zone.
3. Compute zonal failure rate.

Pre-Processor – The Pre-Processor is split into two main sections:

[1] Water pattern creation (working UP the network towards the water main) – The water pattern for every pipe in the independent section of the SCP zone must be evaluated:

- For all Parent-1 Pipes in the independent section
    - Calculate Parent-1 water usage pattern (by effectively combining the water usage patterns of all the connecting SCP houses (children).
- For all Parent-2 Pipes in the independent section
    - Calculate Parent-2 water usage pattern (by effectively combining the water usage patterns of all the connecting Parent-1 Pipes (children).
- Continue until the water usage pattern of the Parent-N Pipe has been calculated.

[2] Computing lead emissions (working DOWN the network towards the houses) – The concentration from each Parent Node must be fed as the input to each of its children in the independent section of the SCP zone:

- For the top-level Parent Pipe (Parent-N Pipe)
    - Compute the concentration at every second in the day at the Parent-N Node.
    - For all Parent-(N-1) Pipes in the independent section.
        - Compute the concentration at every second in the day (using the lead emissions computed for the Parent-N Node as the system input).
        - Continue until lead emissions at all Parent-1 Nodes in the independent section have been evaluated.

3.5.5.2 RDT Sampling

For a house in a standard (non SCP) zone, RDT sampling is simulated by running the model for a single house up to a randomly selected sampling time *ST* and then simulating the collection of a one-litre sample. This simple process can be applied within a SCP zone only if the randomly chosen house is directly connected to the water main, i.e. if it is a non-SCP house. However, if a SCP house is randomly selected within the RDT sampling survey, the corresponding section of the SCP zone must be pre-processed in the same manner as for DAC. For an order-2 SCP zone, this simply involves the pre-processing of the connected Parent-1 Pipe as illustrated (grey component of Figure 3.54).

As with standard (non-SCP) zones, simulations of compliance assessment of SCP zones can be carried out in parallel. However, in this case the most convenient method of dicretising zonal simulations across the available computing resources is to assign each 'slave' CPU a separate independent section of the SCP zone to pre-process and compute lead emissions at the corresponding SCP houses.

3.5.6 Investigating shared communication pipe systems

3.5.6.1 Simple configuration

In order to fully understand the influence of SCPs on household lead emissions it is first necessary to investigate the simplest configuration of a SCP zone, i.e. one single SCP connected to a small number of houses. This simple single-branch configuration is small enough to enable all SCP and household parameters, such as pipe lengths and water usage, to be manually specified and allow for straightforward alterations. In particular, by specifying the length of both the SCP and household pipework, it is possible to adjust the proportion of lead pipework that is shared (% lead shared). To illustrate this concept, a *10m* lead SCP connected to a house having *10m* lead pipework (Figure 3.55) results in *50%* lead shared.

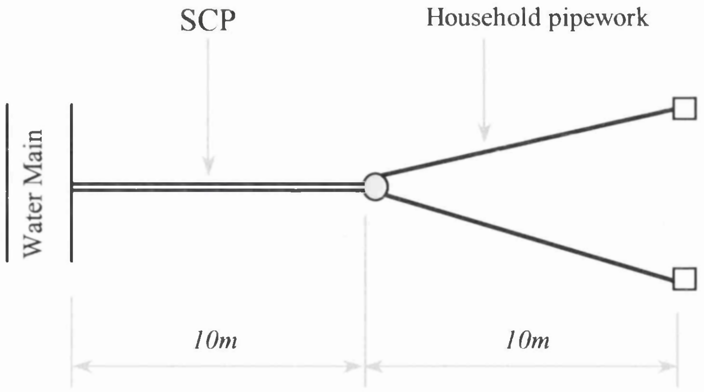


Figure 3.55. Single-branch configuration with 50% lead shared.

Investigation of the influence of SCPs on household lead emissions, in terms of DAC was carried out using a single-branch configuration having a small number of houses (between 2 and 4) supplied through a SCP. Specifically, the influences of the following parameters were examined:

- Length of SCP (expressed as % lead shared)

- Diameter of SCP
- Number of houses supplied through SCP

In each case, the total length of lead pipe used to supply each house is fixed at *20m*, i.e. the length of the household lead pipe plus the length of the SCP is *20m*. This is because the relationship between length of lead pipe and *DAC* is already known (Chapter 2.4.2.2). All other household parameters are fixed at the standard quantities previously defined (Chapter 2.3.1) for each SCP house, except for water usage patterns, which are ascribed as:

House-1:	*30-minute frequency*
House-2:	*15-minute frequency*
House-3:	*7.5-minute frequency*
House-4:	*15-minute frequency*

The purpose of applying different water usage patterns is to avoid the unrealistic scenario of totally concurrent water usage throughout the simulated day. However, it also enables the effect of the water usage pattern to be investigated in a SCP configuration.

Figure 3.56 illustrates how the DAC of House-1 varies with diameter of SCP and % lead shared. These results were obtained using the plug flow – exponential model for a *4*-house configuration, i.e. one SCP supplying water to four houses.

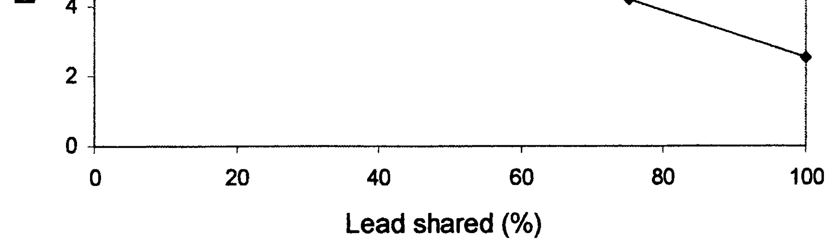


Figure 3.56. Effect of SCP diameter and % lead shared (4-house configuration).

As previously revealed (Chapter 2.4.2.2), the DAC of a non-SCP house increases linearly with length of lead pipe up to lengths of about *100m*, because the lead pipework is the source of the lead emissions that occur at a house. However, in the case of a SCP configuration, the lead emissions arising from the SCP itself are effectively shared between the houses it connects. Consequently, as the proportion of lead pipe that is shared increases, an increasing proportion of the lead emissions become shared. In the most extreme case, when *100%* of the lead pipework is shared (length of SCP = *20m*, length of household lead pipe = *0m*), the DAC is approximately one quarter of its value at *0%* lead shared (length of SCP = *0m*, length of household lead pipe = 2*0m*) for a SCP diameter of *12mm*. This is because all of the lead emissions are now effectively being shared by the four houses connected to the SCP.

Furthermore, as previously revealed (Chapter 2.4.2.4), the DAC of a non-SCP house increases linearly with diameter of pipework, because the surface of area in contact with the given daily volume of water flowing through the lead pipe increases. Thus, the DAC of the SCP houses increase with increasing diameter of SCP.

Figure 3.57 illustrates how the DAC of House-2 varies with number of houses supplied by the SCP and % lead shared. These results were obtained using the plug flow – exponential model for a SCP of diameter *12mm*.

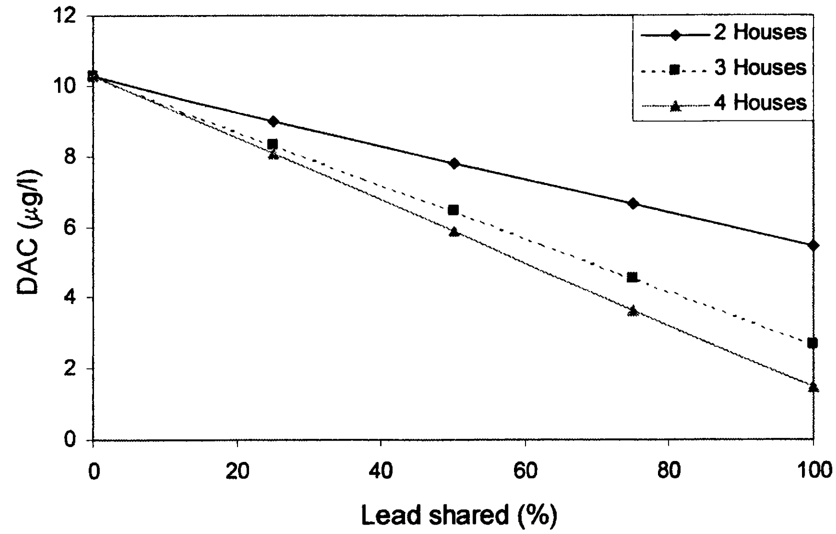


Figure 3.57. Effect of the number of houses supplied by a SCP of 12mm.

Once again, as the proportion of lead pipe that is shared increases, an increasing proportion of the lead emissions from the SCP become shared between the houses it connects. As the number of houses connected to the SCP decreases, the lead emissions from the SCP become shared by fewer houses. Consequently, each house receives a larger share of the lead emissions from the SCP and DAC increases. In the case of two houses, each receives approximately half of the lead emissions resulting from the SCP to which they are connected.

This effect can be combined with the SCP diameter effect, previously discussed, and result in increasing DAC with the % lead shared (Figure 3.58). Indeed, for a SPC configuration of two houses, the DAC is barely affected by the % lead shared when the SCP diameter is *18mm*, and when the SCP diameter is increased to *30mm* the DAC increases significantly with the % lead shared.

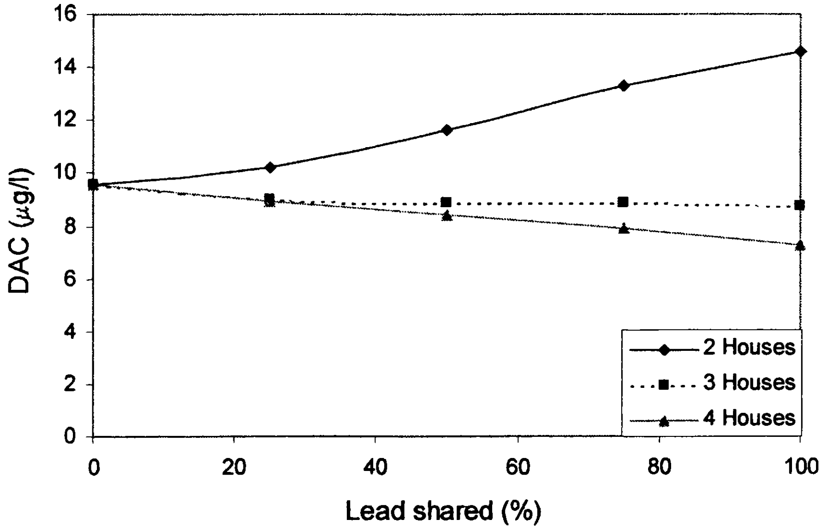


Figure 3.58. Effect of the number of houses supplied by a SCP of 30mm.

3.5.6.2 Effect of SCP on zonal assessment

In order to understand the influence of SCPs on a zonal scale, it is necessary to simulate compliance assessment for several configurations of SCP zones. In the simplest case, this involves comparing the compliance assessment results of a standard (non-SCP) zone to an equivalent zone that has SCPs supplying water to all houses having lead pipework. However, for detail, a number of intermediate zones, where a specified proportion of houses having lead pipework are supplied through SCPs were investigated.

A zone size of *2,000* houses, *40%* of which having lead pipework, was used in each case. Thus, all *800* houses with lead pipework are supplied through a SCP in the case of *100%* SCP. Where present, a SCP effectively replaces a corresponding portion of household lead pipework at the SCP houses it connects, because a separate distribution (Figure 3.52) of reduced lead pipework lengths is applied to the SCP houses.

For each SCP zone, the connections between the SCPs and the houses that they supply are configured by specifying:

- 33% SCP houses share with 1 other SCP house
- 33% SCP houses share with 2 other SCP house
- 33% SCP houses share with 3 other SCP house

Compliance assessment, based on DAC (exact assessment) and RDT at the 10, 25 and 50μg/l standards, was carried out on each zone using the plug flow – exponential model. In the case of a SCP diameter of *12mm*, failure rates based on DAC reduce as the proportion of houses (with lead pipework) that have a SCP increase (Figure 3.59). This trend is evident across each standard, particularly the 10μg/l. Note that the relationships are not completely smooth because of differences in household properties between zones, a result of the random nature inherent in the zone generation process.

These trends can be expected because lead emissions arising from the SCPs within the zone are effectively shared between the houses connected. These houses will therefore experience reduced lead emissions. Consequently, as the proportion of houses (with lead pipework) that have a SCP increase, the proportion of lead emissions that are shared also increases, thus reducing lead emissions and therefore DAC across the zone.

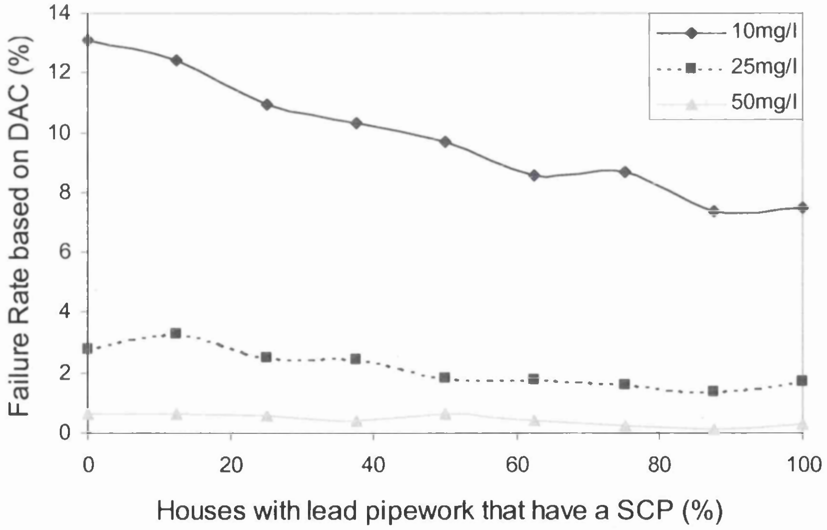


Figure 3.59. Effect of 12mm SCPs on zonal failure rates based on DAC.

A similar relationship is observed for failure rates based on RDT (Figure 3.60), though the magnitude of the effect is smaller.

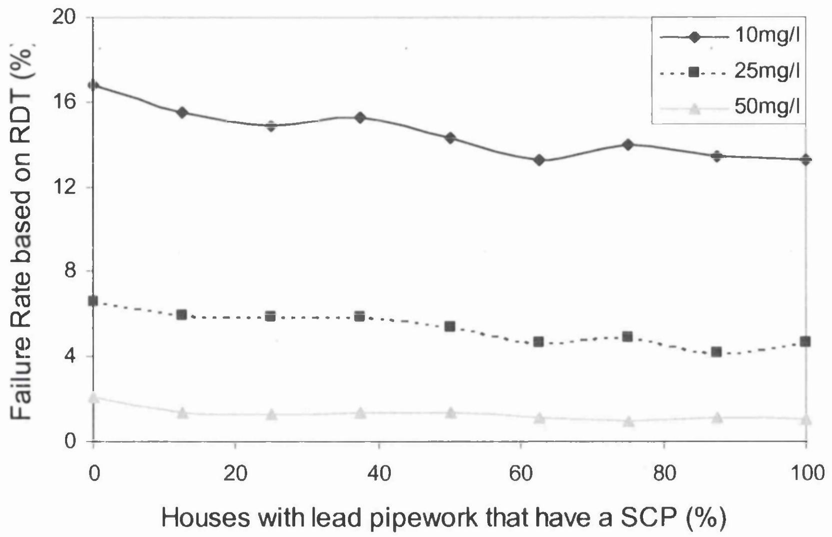


Figure 3.60. Effect of 12mm SCPs on zonal failure rates based on RDT.

The influence of SCP diameter on compliance assessment, based on DAC, is illustrated (Figure 3.61). This shows that zonal failure rates increase with increasing diameter of SCP. This is because the surface of area in contact with the given daily volume of water flowing through the SCP increases with SCP diameter and therefore DAC of the SCP houses also increase. In the case of *30mm* diameter SCP, this effect overcomes the trend of decreasing failure rate with increasing proportion of SCP that is observed for *12mm* diameter SCP, resulting in a slight increase in zonal failure rate with increasing proportion of SCP.

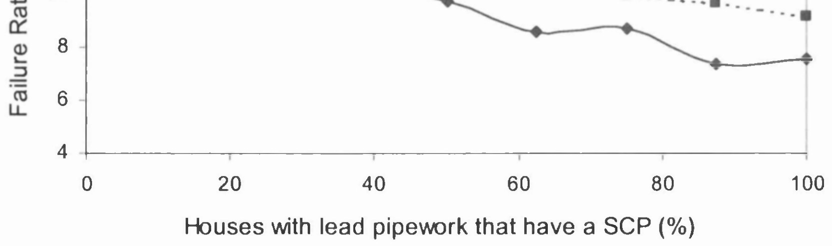


Figure 3.61. Effect of SCP diameter on DAC failure rates against the 10μg/l standard.

4 USING THE MODELS

4.1 Application to real water supply zones

4.1.1 Introduction

As outlined in Chapter 1.1.10, the primary objective of the research described within this thesis is to develop a computational model to assess the compliance of water supply zones with the new lead standards and facilitate the optimisation of corrective treatment. The development of this computational model has been described in detail (Chapter 2 and 3). The model has been used to investigate the effect of household and zonal parameters on lead emissions and zonal compliance assessment (Chapter 3.4). However, these investigations have been limited to the study of pre-defined water supply zones as opposed to real water supply zones. This chapter will describe how the model has been employed to assess the compliance of real water supply zones with the new lead standards and how the model has been used to facilitate the optimisation of corrective treatment. Finally, the computational model will be employed to evaluate the RDT sampling method in terms of how accurately the method predicts actual compliance and the method's suitability for use in the optimisation of corrective treatment.

4.1.2 Validation of model results

Before the model can be confidently employed for assessing compliance and facilitating the optimisation of corrective water treatment of real-world water supply zones, it is necessary to demonstrate that the results from the model are accurate, i.e. are close to corresponding real-world data. In the U.K., the primary real-world data available that relates to lead emissions across a water supply zone is Random Day Time (RDT) sampling survey results, collected by water companies. This is because RDT sampling has been used extensively for assessing compliance with lead standards since 1989 and remains the most favoured protocol in terms of costs, practicality and consumer acceptance, as previously described (Chapter 1.1.9.1). Consequently, validation of the computational model must be carried out by comparing the model results of simulated RDT sampling, in terms of zonal failure rates at various lead standards, with existing RDT sampling results collected from real-world water supply zones by water companies.

In order for the computational model to be confidently employed for facilitating plumbosolvency control on a wide range of zones, validation must be achieved for a number of real-world zones having different water chemistry.

Results from plumbosolvency laboratory testing and appropriate survey data, where available, were obtained for four real water supply zones by Hayes [81]. The data was used by the author to calibrate the zonal model as far as possible, i.e. develop an accurate description of the real water supply zone. The most important calibration factors have been found to be the percentage of properties with lead and the plumbosolvency of the water.

Since RDT sampling is not completely reproducible (Chapter 1.1.9.1), the computational model was used to simulate *100* RDT sampling surveys of *52* samples, and the average zonal failure rate at each lead standard was output.

Where calibration has been satisfactory, good validation between simulated and observed RDT data has been achieved, as illustrated in Table 4.1 for four different water types. Surprisingly, the results from the more simplistic plug flow – exponential model, as opposed to the turbulent – diffusion model, are generally closer to the observed values. In general, discrepancies between the results from the two models at each lead standard are observed to be consistent with previous findings and can be explained in the same manner (Chapter 3.3.3.2).

Table 4.1. Validation of zonal modelling predictions against observed RDT data.

Zone	Model used / observed	Predicted and observed failures rates (%) for RDT sampling against:		
		10μg/l	*25μg/l*	*50μg/l*
	Plug – exponential	27.5	9.9	2.2
A	Turbulent – diffusion	25.9	11.6	0.9
	Observed	28.6	10.2	6.1
	Plug – exponential	11.0	2.9	0.4
B	Turbulent – diffusion	13.9	2.7	0
	Observed	10.0	3.3	1.7
	Plug – exponential	28.8	12.6	3.9
C	Turbulent – diffusion	27.6	14.8	1.8
	Observed	30.0	10.0	2.0
	Plug – exponential	5.9	0.3	0
D	Turbulent – diffusion	5.3	0	0
	Observed	7.1	0	0

Descriptions of zones:

A = Low alkalinity surface water with pH control after physico-chemical treatment but not phosphated.
B = Low alkalinity surface water with pH control after physico-chemical treatment and *0.6 mg/l* (P) phosphate.
C = Blend of high alkalinity groundwaters (limestone bores and springs) with chlorination only.
D = High alkalinity surface water with pH control after physico-chemical treatment and phosphated at *1.0 mg/l* (P).

It should be noted that the results shown in Table 4.1 for Zone B and Zone D relate to treatment conditions prior to the optimisation now required to achieve the new more stringent lead standards. These phosphate-dosing conditions were set to achieve the earlier UK lead standard of *50μg/l* and thus were not optimised for the more stringent *10μg/l* lead standard.

While the single house model has been validated using real-world COMP sampling data, the zonal sampling model has only been validated using RDT sampling data, which has been shown to be less reproducible (22). Additionally, as previously discussed (Chapter 1.1.9.1), a limited number of RDT samples can realistically be taken by a water company in any given year; consequently, yearly observed RDT failure rates are rarely an accurate reflection of the real zonal compliance and often vary significantly from year to year. Thus validation becomes more difficult to demonstrate when the number of RDT sample results, from the water company's sampling, is small.

However, it should be noted that by combining RDT sampling survey data over periods of up to ten years, much of the variation between years is smoothed, thereby minimising the effect of the sampling error and thus improving validation. The observed RDT sampling data illustrated within this chapter typically comprises of approximately 200 samples for each zone. Further investigations using the model have shown that this sample size is sufficient to give a reasonable approximation to the true RDT failure rate. This is illustrated by the results of repeated sampling simulations on Zone-A using a sample size of 200 (Figure 4.1).

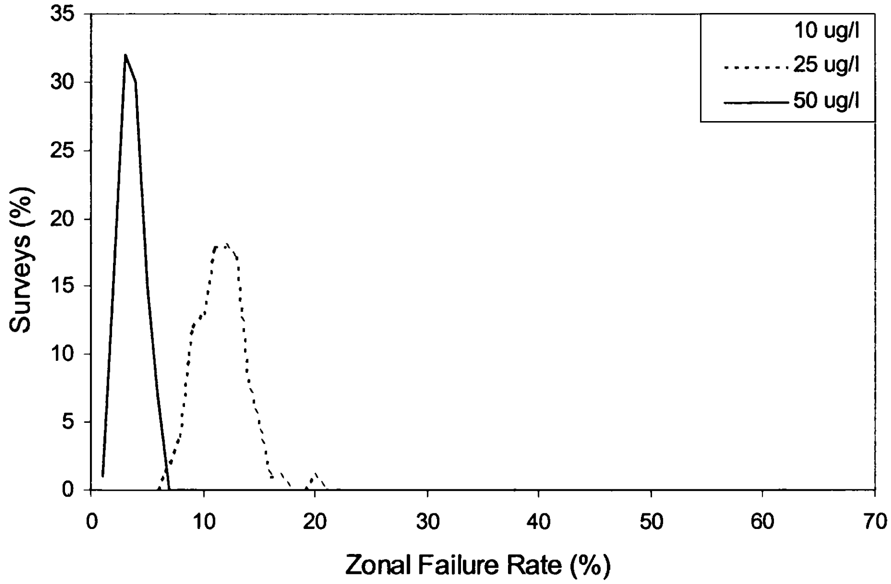


Figure 4.1. Variability in RDT failure rates.

Output from the model shows that an individual sampling survey comprising of 200 samples could in theory give a *10µg/l* zonal failure rate of anywhere between 21 and 36%. However, calculation of the 90% confidence limits reveals that this range reduces to a lowest likely failure rate of 23% and a highest likely failure rate of 33%. From Figure 4.1 it is clear that the confidence interval becomes narrower at the less stringent *25* and *50µg/l* standards, thus providing greater confidence in observed failure rates at these standards.

Subsequent investigation and modelling of real water supply zones across the UK and elsewhere in Europe has been carried out by Hayes [81] using the plug flow - exponential model. This work has formed part of a parallel PhD project undertaken by Hayes [81], focusing more on the application of the model to the regulatory issues of plumbosolvency control than to model development. The results obtained by Hayes show that the degree of fit between predicted and observed RDT failure rates has normally been sufficient to confirm that the zonal model has been calibrated satisfactorily (Table 4.2).

Table 4.2. Further validation of zonal modelling predictions.

Zone	Predicted / Observed	Predicted and observed failures rates for RDT sampling against:		
		10µg/l	*25µg/l*	*50µg/l*
E	Predicted			4.6
	Observed			6.1
F	Predicted	19.5	5.0	0.8
	Observed	9.6	5.8	1.9
G	Predicted	19.6	7.3	1.6
	Observed	18.8	9.4	3.5
H	Predicted	32.4	11.3	2.5
	Observed	40.4	19.9	4.8
I	Predicted	23.1	8.2	1.9
	Observed	23.1	11.1	0.0
J	Predicted	14.7	5.8	1.3
	Observed	14.0	4.0	1.0
K	Predicted	19.5	6.5	1.5
	Observed	22.0	11.0	3.0

In a few cases, however, validation has been poor but further investigations by Hayes [81] have revealed that calibration was wrong. An example is the optimistic calibration of the model for a phosphate dosed zone which was subsequently found to have a poor dosing history, thereby explaining higher observed failure as opposed to the failure predicted [34].

4.1.3 Prediction of actual compliance

After having validated the computational model, using real RDT sampling survey data from water companies, a more comprehensive evaluation of compliance can be carried out for each real-world water supply zone by using the model to simulate 'exact' assessment. This results in a zonal failure rate, at each lead standard, based on the Daily Average Concentration (DAC) of each house within the simulated zone, as previously described (Chapter 3.2.4.1).

Simulation of exact assessment has been carried out for four real-world water supply zones, the properties of which are described in the previous subchapter. Table 4.3 shows the resulting failure rates, comparing the output from the more simplistic exponential – plug flow model to the more exhaustive diffusion – turbulent flow model.

Table 4.3. Model results from simulation of exact assessment.

Zone	Model used	Failure rates (%) for exact assessment (DAC) against:		
		10μg/l	*25μg/l*	*50μg/l*
A	Plug – exponential	20.8	4.6	0.8
	Turbulent – diffusion	27.9	4.2	0.3
B	Plug – exponential	6.7	0.8	0
	Turbulent – diffusion	8.6	0.7	0
C	Plug – exponential	25.4	6.2	1.3
	Turbulent – diffusion	27.1	6.1	0.7
D	Plug – exponential	2.2	0.1	0
	Turbulent – diffusion	1.5	0	0

Zone A, B, C and D Descriptions: as per Table 2.

It can be seen that, in general, the results from the plug flow - exponential model are similar to those from the turbulent – diffusion model. As with the results of RDT sampling, discrepancies between the DAC results from the two models at each lead standard are observed to be consistent with previous findings and can be explained in the same manner (Chapter 3.3.3.1). The largest difference in results between the two models is observed to occur at the *10μg/l* standard, particularly in the case of Zone-A. Although this particular difference appears to be large (Table 1.1), the overall distribution of household DAC across the whole zone for the two models is quite similar (Figure 4.2). However, local differences between these distributions near the "*10μg/l* cut-off" line have a relatively large influence on the *10μg/l* failure rate.

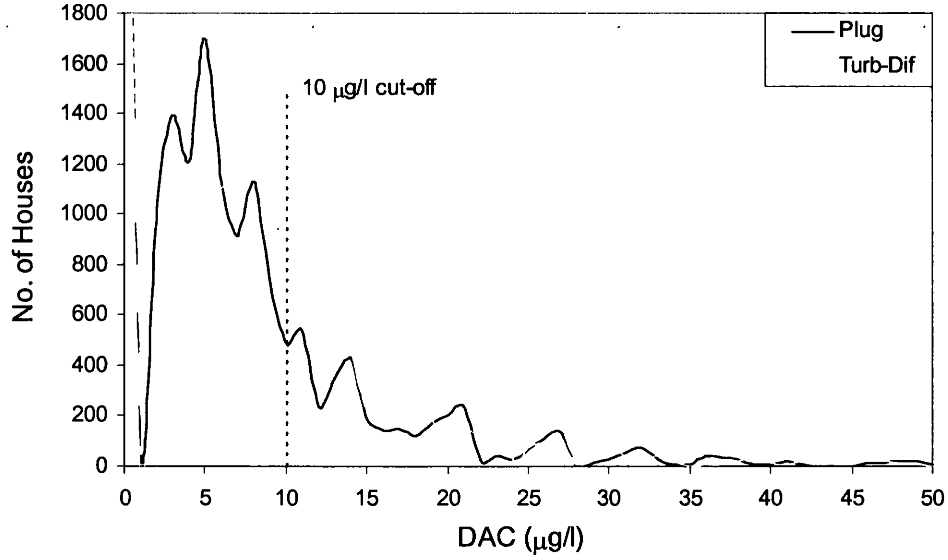


Figure 4.2. Histogram of DAC of houses in Zone-A.

A cumulative histogram for the same DAC data illustrates that the results from the two models only differ noticeably between *2μg/l* and *15μg/l* (Figure 4.3). The absolute difference in failure rates between the two models is similar in this region. However, proportionally, the greatest difference occurs at *9μg/l.*

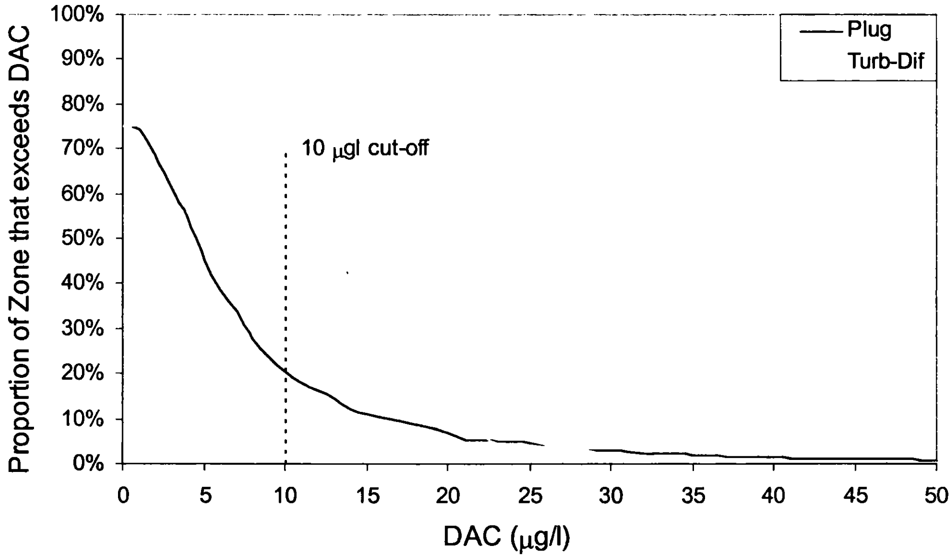


Figure 4.3. Cumulative histogram of DAC of houses in Zone-A.

In general, the results obtained from the simulation of exact assessment are significantly lower than those obtained from the simulation of RDT sampling, previously shown (Table 4.1). This is most apparent in the case of the plug flow – exponential model at each lead standard. These discrepancies are found to be consistent with previous findings and can be explained in the same manner (Chapter 3.3.3.1).

The differences between sampling methods for the plug flow- exponential model can be further illustrated with the distribution of concentration for all houses / samples simulated (Figure 4.4). This illustrates that the distribution of RDT sample concentrations is markedly more skewed towards lower concentrations than the distribution of DAC.

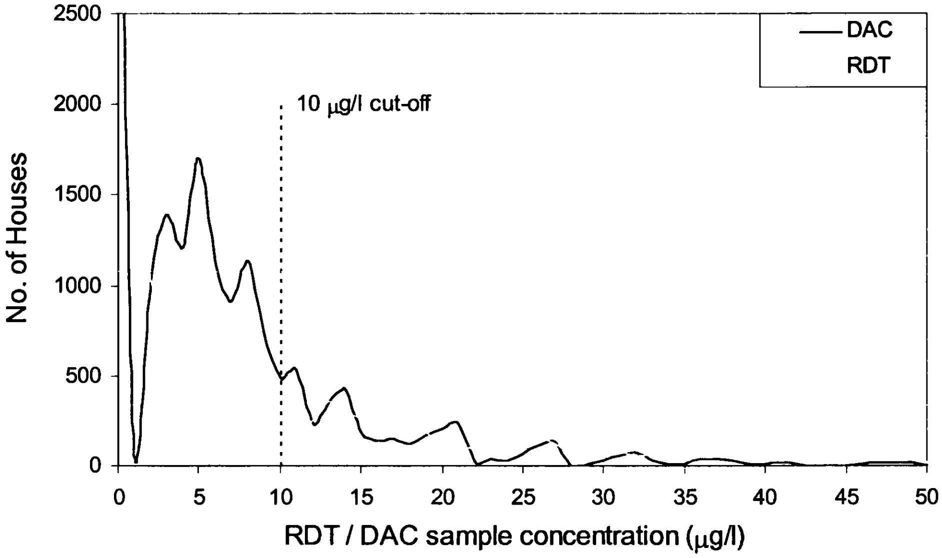


Figure 4.4. Histogram of DAC/RDT sample concentrations in Zone-A.

The significance of the "*10μg/l* cut-off" line can be more clearly explored by considering the cumulative histogram of the same data (Figure 4.5). This clearly illustrates that the difference between RDT and DAC failure rates increases from zero at *7μg/l* to 9% at *14μg/l*, after which it drops to back to zero. Thus, if compliance was measured as failure rate at the *7μg/l* standard, then the RDT and DAC compliance would be the same. However, the proportional difference between the distributions is significant at *10μg/l* and continues to increase up to a concentration of *38 μg/l.*

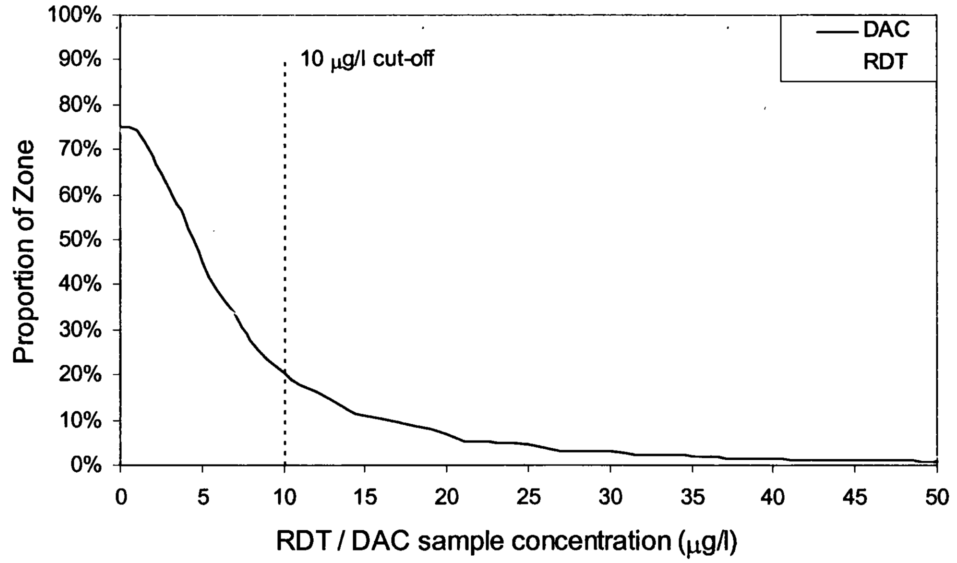


Figure 4.5. Cumulative histogram of DAC/RDT sample concentration in Zone-A.

4.1.4 Rationale for employment of a simplistic model for routine simulations

As discussed in Chapter 2, the lead emissions at a single house can be modelled in varying levels of complexity. The simplest method that has been discussed is the plug flow – exponential model, where the fluid is assumed to be inviscid and the generation of lead within the pipe is described by a simple exponential function. The most complex method discussed is the turbulent – diffusion model, where the fluid is assumed to have viscosity and the generation of lead is described by solutions to the classical equations of mass transfer.

Although the plug flow – exponential model is not as physically accurate as the turbulent – diffusion model, it is computationally much faster to execute as it is more straightforward mathematically and does not require radial discretisation of pipework. Indeed, through the use of the plug flow – exponential model, it is possible to perform large zonal simulations on modest computing resources. Furthermore, there is little point modelling the physical processes in great detail if basic parameters, such as length of pipework and daily water consumption, are not accurately known. However, the employment of this simplistic model for routine simulations can only be justified if validation with real world data as well as equivalent results from the more complex turbulent – diffusion model can be demonstrated.

Results for a single house, in terms of the daily variation of lead emissions, have been obtained for both the plug flow – exponential and the turbulent – diffusion model (Chapter 2.3). Analysis of the variation of lead emissions with time during a single flow event has revealed that the plug flow – exponential model approximates well to the turbulent – diffusion model for a typical flow event assuming normal household circumstances, i.e. *10m* length of lead pipe, *Q = 0.1 l/s* (Figure 2.24). Subsequent sensitivity analyses of household circumstances have revealed that the two models behave similarly with the only discernable differences occurring when the diameter of the pipework is large or when the inter-use time is very small (Chapter 2.4).

Validation of DAC results for both plug flow – exponential and turbulent – diffusion models has been successfully demonstrated for a wide range of different household circumstances by comparing model results to those obtained from published composite proportional (COMP) sampling data from actual COMP sampling surveys (Chapter 2.4.1). Consequently, the plug flow - exponential model can be confidently employed for investigating lead emissions at a single house.

Results for a water supply zone, in terms of the zonal failure rates at the *10, 25* and *50μg/l* standards, based on various sampling protocols, have also been obtained for both the plug flow – exponential and the turbulent – diffusion model (Chapter 3.3). This has revealed very little difference between the two models at each lead standard for both DAC and RDT simulations. Additionally, validation of the zonal model has been carried out for both the plug flow – exponential model and the turbulent – diffusion model. Where calibration has been satisfactory, good validation between simulated and observed RDT data has been achieved (Table 4.1). Surprisingly, the results from the more simplistic plug flow – exponential model, as opposed to the turbulent – diffusion model, are generally closer to the observed values. Consequently, the plug flow - exponential model can be confidently employed for assessing the compliance of real water supply zones and facilitating the optimisation of corrective treatment.

Thus, it has been demonstrated that the computationally faster plug flow – exponential model is a suitable approximation to the more complex turbulent – diffusion model and its application within a computational model for routine zonal simulations is justified. This satisfies a primary aim of this research, namely to develop a computational model that can run on modest computing resources, i.e. a standard PC rather than a supercomputer.

4.1.5 Optimisation of corrective treatment

4.1.5.1 Introduction

One of the primary applications of the computational model is to investigate the likely effects of corrective water treatment and selective lead pipe replacement. This is intended to facilitate the optimisation of plumbosolvency control measures and substantially overcome the severe limitations of traditional sampling. As previously shown, the computational model has been satisfactorily validated for a wide range of water types, permitting the procedure to investigate treatment scenarios with confidence.

The most effective corrective water treatment technique is dosing of phosphate (a corrosion inhibitor) at an appropriate pH, as previously described (Chapter 1.1.8.2). In order to investigate the effects of corrective treatment in a real water supply zone, it is necessary to develop an accurate zonal description of that water supply zone. This is achieved through calibration with reference to:

- the results from laboratory plumbosolvency testing for pre-phosphate dosing conditions; and results from post-phosphate dosing, if available.
- observed reductions in lead emissions at reference houses and lead pipe rigs; and
- surveys of houses with lead pipework (length, diameter, consumer behaviour) [80].

Optimisation of corrective water treatment can be investigated to a higher degree of confidence when good validation is achieved for both pre- and post-phosphate dosing conditions.

The plumbosolvency of the water is defined by the equilibrium solubility E and the diffusion coefficient D for the diffusion model, or M for the exponential approximation, as previously discussed (Chapter 2.2.3). It is possible to simulate water treatment simply by controlling the D and E, or M and E parameters used to describe the water supply zone being investigated. Thus, by simulating RDT sampling surveys for a range of plumbosolvency reductions, it is possible to determine the target plumbosolvency, and therefore the target percentage reduction in initial plumbosolvency, required to achieve a specified compliance.

4.1.5.2 Real-world example

In order to fully illustrate the application of the computational model to the optimisation of corrective water treatment, a real-world example [81] is described. The example relates to a real water supply zone in South England.

The objective of the study is to investigate the potential effectiveness of phosphate dosing and to determine the likely feasibility of the selective replacement of lead pipes in the zone. Additionally, to assess the likely effectiveness of the blanket removal of the lead communication pipes owned by the water company.

The water supply zone has the following characteristics:

- Water type: The zone is fed by a mixture of spring water and limestone groundwater, via a single reservoir. The water is slightly alkaline, has a high alkalinity and a low organic content. It is not phosphate dosed.

- Plumbosolvency: Moderate when water is untreated. From laboratory testing, the plumbosolvency parameters are found to be:
  $M = 0.106\ \mu g/m^2/sec$
  $E = 242\mu g/l$

- Total number of houses in the water supply zone: *14,787.*
- Percentage of houses estimated that have a lead pipe: *68%*

These parameters are used to generate a detailed description of the 'untreated' water supply zone for the subsequent simulation of compliance assessment. It should be noted that the zonal distributions of household parameters, such as pipework length and water consumption, are described by the standard zonal assumptions previously described (Chapter 3.2.1).

Additional zones are generated using the same parameters as those that describe the 'untreated zone' with the exception of the plumbosolvency parameters, which are progressively reduced. Thus, each zone represents a degree of simulated water treatment.

4.1.5.3 Validation of results

Before the computational model is used to predict the likely effects of water treatment, validation between the model results and actual RDT sampling survey results for the 'untreated' zone must be demonstrated. Since *RDT* sampling survey results are never completely reproducible, the simulated survey is repeated *100* times and an average failure rate at each lead standard is computed. Good validation is illustrated for both the plug flow – exponential and the turbulent – diffusion models for the *10*, *25* and *50*$\mu g/l$ lead standards (Table 4.4).

Table 4.4. Validation of zonal modelling predictions against observed RDT data.

Model used / observed	**Predicted and observed failures rates for RDT sampling against:**		
	10μg/l	***25μg/l***	***50μg/l***
Plug – exponential	28.8	12.6	3.9
Turbulent – diffusion	27.6	14.8	1.8
Observed *	30.0	10.0	2.0

* Values quoted by the water company, based on *379* samples collected over a *10*-year period.

4.1.5.4 Prediction of the effects of water treatment

It is concluded that the model is validated sufficiently to enable it to be used as a tool to predict the effects of water treatment and subsequent optimisation of water treatment for this water supply zone. RDT sampling surveys can now be simulated on the 'treated' zones, previously generated. The results, generated using the plug flow – exponential model, in terms of failure rates at each lead standard are illustrated for each degree of water treatment, including the 'untreated' zone (Table 4.5).

Table 4.5. Model results from simulation of RDT sampling (water treatment).

Plumbosolvency Reduction (%)	***M*** ***($\mu g/m^2/sec$)***	**E** ***(μg/l)***	**Failure rates for RDT sampling against:**		
			10μg/l	***25μg/l***	***50μg/l***
0	0.106	242.0	28.84	12.57	3.94
50	0.053	121.0	15.87	3.54	0.48
60	0.042	96.8	13.05	2.10	0.15
70	0.032	72.6	7.83	0.87	0.03
80	0.021	48.4	3.82	0.21	0.00
90	0.011	24.2	0.59	0.00	0.00

The results clearly illustrate how the failure rates at each lead standard reduce as the degree of treatment is increased, i.e. as the plumbosolvency is reduced. On the basis of historic RDT data, the trigger for action set by the Drinking Water Inspectorate [32,33] was *5%* failure against the *10μg/l* standard. From Table 4.5 it is observed that an *80%* reduction in plumbosolvency results in a failure rate, at the *10μg/l* standard, of *3.8%*, i.e. below the trigger value. Furthermore, it is observed that a *90%* reduction in plumbosolvency results in a failure rate of *0.59%*, i.e. *87* houses at the *10μg/l* standard and no houses failing the less stringent *25μg/l* and *50μg/l* standards.

In addition to RDT sampling, exact compliance can be simulated on the 'untreated' and 'treated' zones, previously generated. The results, in terms of failure rates at each lead standard, based on the Daily Average Concentration (DAC) of all houses within the zone, are illustrated for each degree of water treatment, including the 'untreated' zone (Table 4.6).

Table 4.6. Model results from simulation of exact assessment (water treatment).

Plumbosolvency reduction (%)	***M*** *($\mu g/m^2/sec$)*	**E** *($\mu g/l$)*	**Failure rates for exact compliance (DAC) against:**		
			10μg/l	*25μg/l*	*50μg/l*
0	0.106	242.0	25.37	6.34	1.32
50	0.053	121.0	9.94	1.31	0.09
60	0.042	96.8	6.23	0.83	0.05
70	0.032	72.6	2.96	0.32	0.01
80	0.021	48.4	1.31	0.05	0.00
90	0.011	24.2	0.09	0.00	0.00

Once again, the results clearly illustrate how the failure rates at each lead standard reduce as the degree of treatment is increased, i.e. as the plumbosolvency is reduced. However, it should be noted that the failure rates based on DAC are significantly lower than those based on RDT. This observation is consistent with previous findings (Chapter 3.3.3.1).

By analysing the detailed output data from the simulation of exact compliance, it is possible to determine the characteristics of the 'problem' houses, i.e. the houses that have the highest DAC and continue to fail the *10μg/l* standard when the plumbosolvency has been reduced by *80%*. From Table 4.6 it is observed that an *80%* reduction in plumbosolvency results in a failure rate of *1.31%*, i.e. *194* houses at the *10μg/l* standard. Of these *194* problem houses, the maximum daily water consumption is *150 litres* and the minimum length of lead pipework is found to be *40m* for households having daily water consumption of *150 litres* (i.e. single residency).

It is encouraging to note here that *80%* reductions in plumbosolvency have already been readily achieved operationally by phosphate dosing for a range in water types across the UK, as judged by fixed point bench-marking using 30MS samples, examples being Bristol, Cambridge and Exeter [34]. It is anticipated that optimisation of corrective water treatment can achieve at least *85%* reductions in plumbosolvency in most water supply zones.

Through the use of computational modelling, it has been predicted that corrective water treatment alone will achieve zonal compliance with the new lead standards in most water supply zones. From the application of this modelling technique, a simple method of operational control now becomes possible, in which the target band in the percentage reduction in plumbosolvency, as determined by computational modelling, can be monitored by 30MS sampling at bench-marking houses (for as long as they are available) and lead pipe test rigs, as illustrated (Figure 4.6) [34].

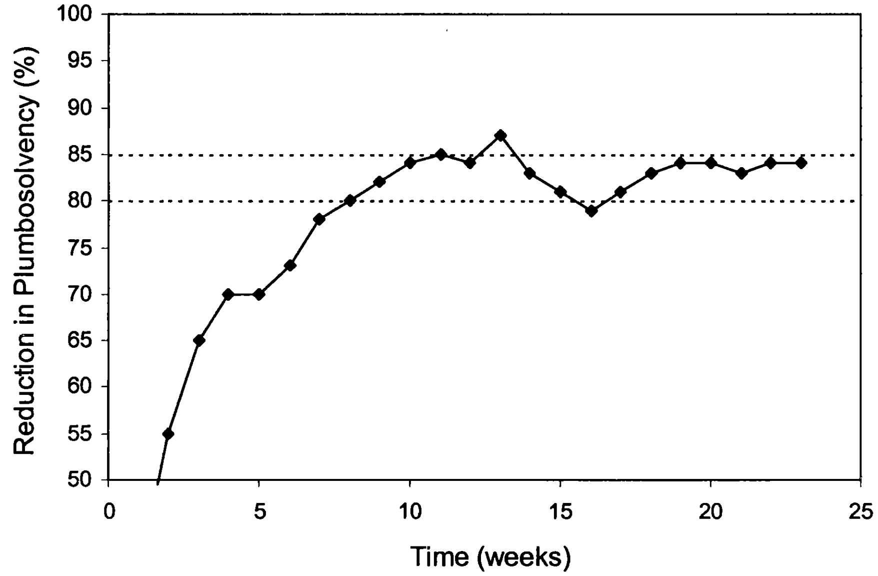


Figure 4.6. Example of plumbosolvency reduction during operational control.

4.1.5.5 Prediction of the effects of lead pipe replacement

In addition to simulating the effects of corrective water treatment, the computational model may also be used to simulate the effects of lead pipe replacement that may occur during the blanket removal of the lead communication pipes owned by the water company.

In this case, additional zones are generated using the same parameters as those that describe the 'untreated zone' with the exception of the distribution of lead pipework lengths, the values of which are progressively reduced. Thus, each zone represents a degree of simulated lead pipe replacement.

As before, RDT sampling as well as exact compliance can be simulated on the 'lead pipe reduced' zones previously generated. The results, generated using the plug flow – exponential model, in terms of failure rates at each lead standard are illustrated for each degree of water treatment, including the 'untreated' zone (Table 4.7 and Table 4.8).

Table 4.7. Model results from simulation of RDT sampling (lead pipe replacement).

Reduction in length of all lead pipework within zone (m)	M ($\mu g/m^2/sec$)	E ($\mu g/l$)	Failure rates for RDT sampling against:		
			10μg/l	25μg/l	50μg/l
0	0.106	242.0	28.84	12.57	3.94
5	0.106	242.0	21.54	7.98	2.23
10	0.106	242.0	15.18	5.22	1.33

Table 4.8. Model results from simulation of exact assessment (lead pipe replacement).

Reduction in length of all lead pipework within zone (m)	*M* ($\mu g/m^2/sec$)	E ($\mu g/l$)	Failure rates for exact compliance (DAC) against:		
			10μg/l	*25μg/l*	*50μg/l*
0	0.106	242.0	25.37	6.34	1.32
5	0.106	242.0	16.14	3.78	0.87
10	0.106	242.0	9.66	2.25	0.44

From both sets of results it is clear that lead pipe replacement is considerably less effective than water treatment at reducing lead emissions. Indeed, even with a *10m* reduction in all lead pipework length, the zonal failure rates from both RDT sampling and exact compliance greatly exceed the trigger value for action set by the Drinking Water Inspectorate of *5%* failure against the *10μg/l* standard.

Thus, blanket removal of lead communication pipes by itself, to meet the new lead standards, is clearly not a viable option considering the huge cost and disruption that would result from replacement of lead pipework on a zonal scale, previously described (Chapter 1.1.8.1). However, selective lead pipe replacement combined with corrective water treatment for the purposes of reducing zonal failure rates is feasible. In this case, any lead pipe replacement will have to be selective and strategic, this will usually be where lead concentrations in consumer's drinking water are highest. Such 'problem' houses can be identified from the likely characteristics of houses having the greatest DAC, as determined from the simulation of exact compliance, previously described (Chapter 4.1.6.7).

4.1.6 Shared Communication Pipes Case Study

4.1.6.1 Introduction

It has previously been explained how the computational model has been used to investigate the likely effects of corrective water treatment in a real water supply zone within the U.K. for the purposes of assisting the optimisation of water treatment (Chapter 4.1.4). This zone was treated as a number of houses that are individually connected to the water mains by a single communication pipe. This is usually an accurate representation of a water supply zone in the U.K. because very few zones have large proportions of apartment blocks or flats. However, it has been found that the housing in some European cities is predominantly connected through SCPs (Shared Communication Pipes) [61], particularly where houses are terraced and adjacent to the road, i.e. have no front garden.

In order to fully illustrate the application of the computational model to the optimisation of corrective water treatment in a zone having SCPs, a real-world example [82] is described. The example relates to a real water supply zone in a provincial West European city.

The objective of the study is to generate an accurate description of the water supply zone from existing survey data and to validate simulated compliance results with observed results. Additionally, to investigate the potential effectiveness of phosphate dosing, if validation is demonstrated.

4.1.6.2 General characteristics of water supply zone

The water supply zone has the following general characteristics:

- Water type: Moderately plumbosolvent water that is not phosphate dosed.
- Plumbosolvency: From laboratory testing, the plumbosolvency parameters are found to be:
  $M = 0.072\ \mu g/m^2/sec$
  $E = 145 \mu g/l$
- The number of dwellings within the zone is unknown. However, the population of the water supply zone has been estimated as: *278,500* people.
- Total daily water consumption in zone: *33.4 Mlitres*. This results in an average daily consumption of water per person of approximately *120 litres.*

Since the connectivity in a real SCP zone is often largely unknown, it is necessary to assume the general structure of the zone in terms of the hierarchy of SCPs. The water supply zone is assumed to comprise of three different types of dwellings, which are treated as follows:

- Single dwellings – do not share communication pipes with other dwellings and can be treated as independent. Main communication pipe connects the single dwelling directly to the water main.

- Flats within a small block – share a main communication pipe with all other flats in the block. Main communication pipe connects each flat in the block to the water main.

- Flats within a large block – share communication pipes with other flats on the same floor of the block. Communication pipes on each floor of the block connect to a larger main communication pipe, which connects to the water main

4.1.6.3 Water consumption

Survey data from the water company relates to the length and daily water throughput for the main communication pipes, i.e. the pipes that directly connect to the water main. By utilising the survey data for daily water throughput and applying the condition that the total throughput of all the main communication pipes within the zone must equal *33.4 Mlitres*, the distribution of daily throughput per main communication pipes has been estimated (Light bars in Figure 4.7).

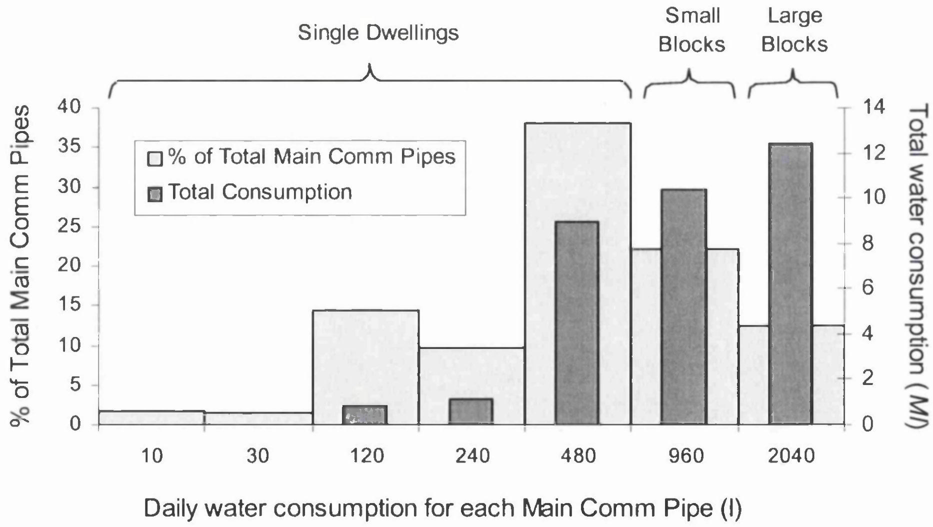


Figure 4.7. Distribution of daily water throughput of Main Communication Pipes.

Additionally, the total water throughput for all main communication pipes in each band is calculated by multiplying the daily water throughput per main communication pipe by the associated *%* of total (Dark bars in Figure 4.7). Since the average daily consumption of water per person is approximately *120 litres*, an equivalent occupancy can be calculated for each band of daily throughput per main communication pipe. Thus, the zone is broken down in terms of dwellings as follows:

- Single dwellings: Daily water consumption varies from *10* to *480 litres*. This results in an equivalent occupancy of *1 – 4* occupants. The resulting distribution of daily water consumption for single dwellings is illustrated (Figure 4.8a).

- Small blocks of flats: Daily water consumption is *960 litres*, relating to an equivalent occupancy of *8* occupants. The number of individual flats in each small block is assumed to be *3* as this would result in an average occupancy per flat of *2.7*, which is plausible. This assumption results in an average daily water consumption of *320 litres* per flat.

- Large blocks of flats: Daily water consumption is *2040 litres*, relating to an equivalent occupancy of *17* occupants. The number of individual flats in each large block is assumed to be *6* as this would result in an average occupancy per flat of *2.8*, which is plausible. This assumption results in an average daily water consumption of *340 litres* per flat.

For simplicity, the average daily water consumption for flats in both small and large blocks is taken to be *330 litres*. In order to take into account the variation in water consumption that would occur across the zone, a simple uniform distribution, based around the average daily water consumption, is assumed for both flats in small blocks and flats in large blocks (Figure 4.8b).

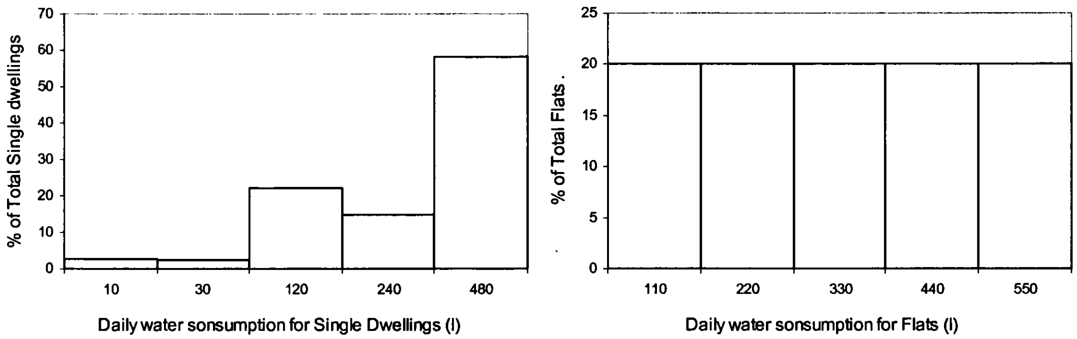


Figure 4.8. Distribution of daily water consumption for a) Flats and b) Single Dwellings.

As there is no survey data that relates to the pattern of water usage, the standard patterns, previously described (Chapter 2.2.2), will be employed.

4.1.6.4 Configuration of zone

As previously discussed, the water supply zone is assumed to comprise of three different types of dwellings, namely single dwellings, flats in small blocks and flats in large blocks. By observing the total consumptions for each type of dwelling (Figure 4.7), it is clear that approximately one third of all dwellings within the zone are single dwellings, one third are flats in small blocks and one third are flats within large blocks. Again, this is a reasonable assumption considering the zone is within a large provincial city.

For simplicity, it is assumed that small blocks comprise one floor having *3* flats and large blocks comprise two floors having *3* flats on each floor. The resulting configuration of the zone in terms of connectivity is illustrated (Figure 4.9).

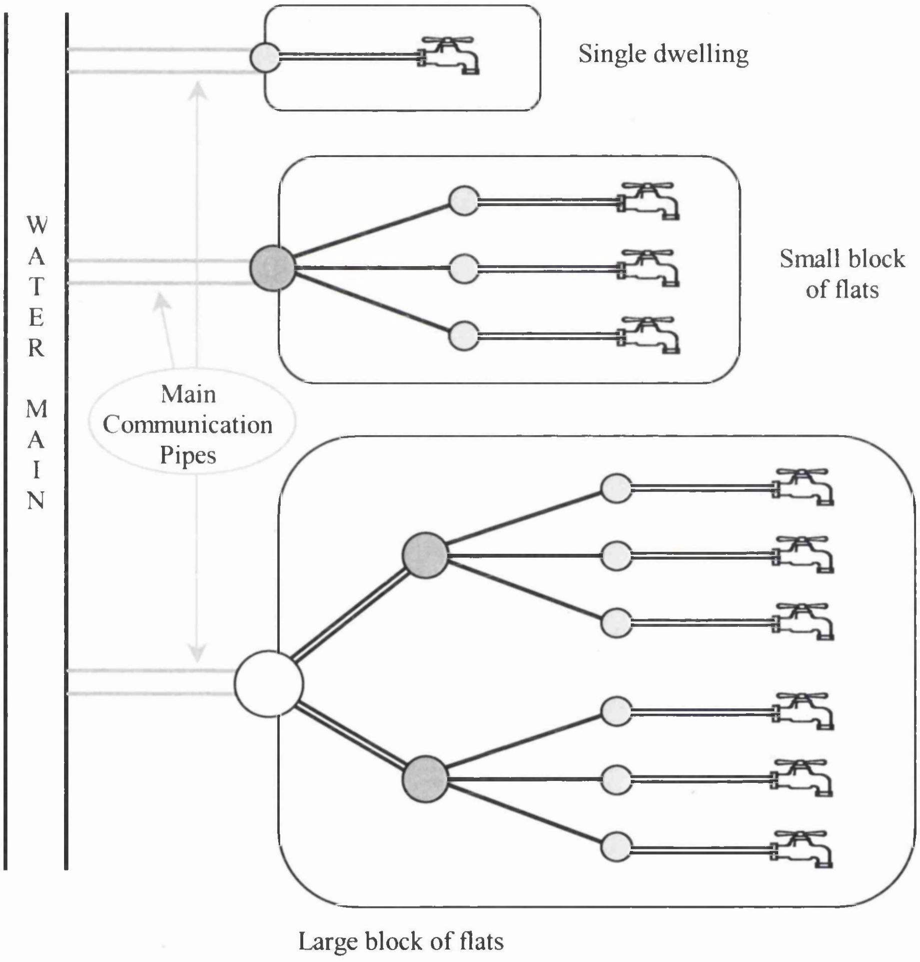


Figure 4.9. Connectivity in zone.

4.1.6.5 Pipework

The distribution of the lengths of the main communication pipes within the zone, obtained from survey data from the water company, is illustrated (Figure 4.10). It should be noted that this distribution includes both lead and non-lead communication pipes. However, the water company estimates that *23.5%* of all main communication pipes are made from lead. For simplicity, it is assumed that where a single dwelling or block of flats is supplied through a main communication pipe that is made from lead, the pipework within the single dwelling or block of flats is also made from lead.

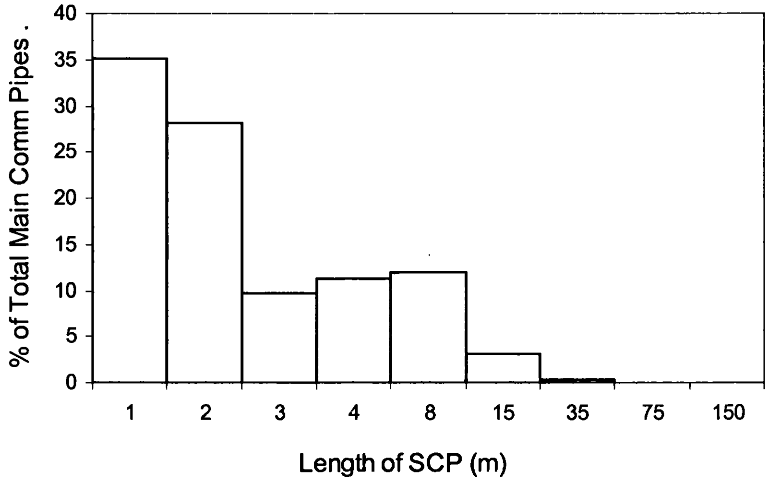


Figure 4.10. Distribution of length of Main Communication Pipes.

There is no survey data that relates to lengths of pipework within dwellings or flats; consequently, a basic distribution has been assumed, with mean *10m*. Additionally, since there is no survey data relating to SCPs within large blocks of flats (the pipes that connect the flats to the main communication pipe supplying the block), a basic distribution has been assumed (Figure 4.11). This distribution has a higher mean length in order to reflect the longer pipework necessary to span the longer distances that will occur in large blocks of flats.

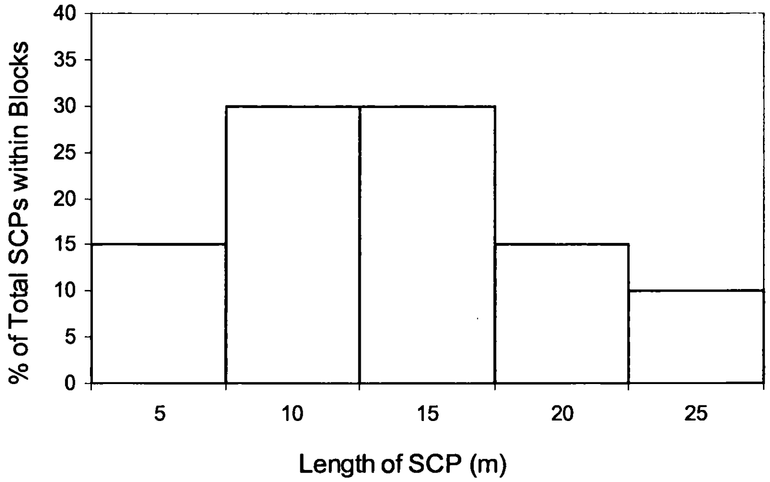


Figure 4.11. Distribution of length of Shared Communication Pipes.

The diameter of plumbing within all single dwellings and flats is assumed to be *18mm*. However, diameters of SCPs, in particular main communication pipes that supply large blocks of flats, are likely to be significantly greater. Survey data from the water company suggests:

- Diameter of main communication pipes supplying single dwellings: *25mm*.
- Diameter of main communication pipes supplying small blocks of flats: *25mm*.
- Diameter of SCPs within large blocks of flats: *25mm*.
- Diameter of main communication pipes supplying large blocks of flats: *38mm*.

The general zonal characteristics, connectivity and assumed distributions of pipework lengths and water usage are used to generate a detailed description of the 'untreated' water supply zone for the subsequent simulation of compliance assessment.

Additional zones are generated using the same parameters as those that describe the 'untreated zone' with the exception of the plumbosolvency parameters, which are progressively reduced. Thus, each zone represents a degree of simulated water treatment.

4.1.6.6 Validation of results

Before the computational model is used to predict the likely effects of water treatment, validation between the model results and actual RDT sampling survey results for the 'untreated' zone must be demonstrated. Since *RDT* sampling survey results are never completely reproducible, the simulated survey is repeated *100* times and an average failure rate at each lead standard is computed. Good validation is illustrated for both the plug flow – exponential and the turbulent – diffusion models for the *10*, *25* and *50μg/l* lead standards (Table 4.9).

Table 4.9. Validation of zonal modelling predictions against observed RDT data.

Model used / observed	**Predicted and observed failures rates for RDT sampling against:**		
	10μg/l	***25μg/l***	***50μg/l***
Plug – exponential	19.0	8.5	1.9
Turbulent – diffusion	15.9	6.6	1.6
Observed *	19.6	6.5	2.2

* Values quoted by the water company, based on *46* samples.

The results from the plug flow – exponential model are found to be higher than those from the turbulent – diffusion model. This is because the exponential model over estimates the concentration of lead in larger diameter pipes, as previously discussed (Chapter 2.4.2.4). Additionally, it should be noted that the observed RDT survey results are based on only *46* samples and are thus highly speculative due to the considerable sampling error.

4.1.6.7 Prediction of the effects of water treatment

It is concluded that the model is validated as far as possible to enable it to be used as a tool to predict the effects of water treatment and subsequent optimisation of water treatment for this water supply zone. RDT sampling surveys can now be simulated on the 'treated' zones, previously generated. The results, generated using the plug flow – exponential model, in terms of failure rates at each lead standard are illustrated for each degree of water treatment, including the 'untreated' zone (Table 4.10).

Table 4.10. Model results from simulation of RDT sampling.

Plumbosolvency Reduction (%)	***M*** ***(μg/m²/sec)***	**E** ***(μg/l)***	**Failure rates for RDT sampling against:**		
			10μg/l	***25μg/l***	***50μg/l***
0	145.0	0.0720	18.97	8.47	1.88
50	72.5	0.0360	12.04	2.32	0.26
60	58.0	0.0288	8.53	1.11	0.14
70	43.5	0.0216	5.84	0.36	0.00
80	29.0	0.0144	2.18	0.15	0.00
85	22.0	0.0108	0.75	0.00	0.00

As in the previous case study, the results clearly illustrate how the failure rates at each lead standard reduce as the degree of treatment is increased, i.e. as the plumbosolvency is reduced. On the basis of historic RDT data, the trigger for action set by the Drinking Water Inspectorate [32,33] was *5%* failure against the *10μg/l* standard. From Table 4.10 it is observed that an *80%* reduction in plumbosolvency results in a failure rate, at the *10μg/l* standard, of *2.18%*, which is significantly below the trigger value. Furthermore, it is observed that an *85%* reduction in plumbosolvency results in a failure rate of *0.75%*, i.e. *756* dwellings at the *10μg/l* standard and no dwellings failing the less stringent *25μg/l* and *50μg/l* standards.

In addition to RDT sampling, exact compliance can be simulated on the 'untreated' and 'treated' zones, previously generated. The results, in terms of failure rates at each lead standard, based on the Daily Average Concentration (DAC) of all dwellings within the zone, are illustrated for each degree of water treatment, including the 'untreated' zone (Table 4.11).

Table 4.11. Model results from simulation of exact assessment.

Plumbosolvency reduction (%)	*M* *(μg/m²/sec)*	E *(μg/l)*	Failure rates for exact compliance (DAC) against:		
			10μg/l	*25μg/l*	*50μg/l*
0	145.0	0.0720	18.13	5.11	0.48
50	72.5	0.0360	7.85	0.48	0.22
60	58.0	0.0288	5.11	0.43	0.20
70	43.5	0.0216	2.49	0.30	0.00
80	29.0	0.0144	0.48	0.20	0.00
85	22.0	0.0108	0.41	0.00	0.00

Once again, the results clearly illustrate how the failure rates at each lead standard reduce as the degree of treatment is increased, i.e. as the plumbosolvency is reduced. However, it should be noted that the failure rates based on DAC are significantly lower than those based on RDT. This observation is consistent with previous findings (Chapter 3.3.3.1).

By analysing the detailed output data from the simulation of exact compliance, it is possible to determine the characteristics of the 'problem' dwellings, i.e. the dwellings that have the highest DAC and continue to fail the *10μg/l* standard when the plumbosolvency has been reduced by *85%*, this reduction being deemed operationally achievable [61]. From Table 4.11 it is observed that an *85%* reduction in plumbosolvency results in a failure rate of *0.41%*, i.e. *413* dwellings at the *10μg/l* standard. All of the *413* problem dwellings are found to be single dwellings; only ten of which had daily water consumption greater than *120 litres* (i.e. single residency). This observation is highly significant as it enables the water company to easily identify problem dwellings for the purposes of selective lead pipe replacement after corrective treatment has been optimised.

4.2 Statistical investigation of RDT sampling

4.2.1 Introduction

The revised European Union (1998) "drinking water" directive [30] requires Member States to comply with a lead standard of *25μg/l* by December 2003 and then *10μg/l* within a further ten years, these limits being related to the weekly average concentration at individual properties. The Directive requires compliance samples, in respect of the lead parameter, to be taken from the point of use by consumers (normally taken to be the kitchen tap), although a harmonised sampling method has yet to be specified.

In the UK, it is anticipated that random daytime sampling will be used for demonstrating compliance with the new lead standards, this approach having been used since 1989 for assessing compliance with the current lead standard of *50 μg/l*. Such sampling comprises:

- visiting a consumer's house that has been selected randomly (if access is not possible then the house next door is tried, and so on, until access is gained)
- the visit is made at any time of the day within normal working hours (i.e. about *0900* to *1700* hours)
- the sample taken is the first litre drawn from the kitchen cold water tap without prior flushing.

In respect of the lead parameter, the minimum sampling frequencies specified by the UK Water Supply Regulations (that implement the Directive) vary from only *1* to *8* samples per year from each water supply zone, dependent on the population involved (up to a maximum of *100,000* people). It is widely recognised that such frequencies are far too low for accurate assessments to be made. However, the random daytime sampling of water supply zones is more comprehensive in respect of assessing compliance with bacteriological standards, the minimum specified sampling frequencies varying from *12* to *240* per year for zones serving up to *100,000* people.

In the UK, the preferred approach of the Drinking Water Inspectorate, for endeavouring to comply with the new lead standards comprises:

- corrective water treatment by dosing phosphate at an appropriate pH
- optimisation of the phosphate dose to achieve the maximum practicable reductions in lead emissions

- selective replacement of lead pipes that fail to respond to optimised zone-wide treatment, as far as this may be necessary.

The UK's Drinking Water Inspectorate (DWI) has issued two Information Letters [32,33] in the past two years that require water companies to monitor their water supplies in relation to the optimisation of the plumbosolvency treatment measures that they have taken. The DWI has indicated a clear preference that water companies should undertake such monitoring at fixed points (i.e. benchmarking points) using either representative reference houses which have a lead pipe or suitably located lead pipe test rigs. The DWI will only permit a water company to use random daytime sampling for the purposes of optimising plumbosolvency control if it can be demonstrated that such sampling is equivalent to the monitoring of fixed reference points. This is because it is believed [22,48] that random daytime sampling is insufficiently reproducible. However, the use of random daytime sampling for this purpose is favoured by some water companies, because it is less inconvenient for customers, less costly and it would be most opportune to take samples for lead analysis in conjunction with the more extensive bacteriological monitoring that is carried out.

Generally, when water is first treated by the addition of phosphate, the plumbosolvency (a measure of the extent of lead dissolution) of the water will be reduced considerably, typically by *60* to *70%*. Consequently, the reduction in lead emissions should be easier to demonstrate. However, it is likely to be harder to quantify subsequent improvements during the optimisation stage of treatment because the reductions in plumbosolvency will be much smaller (Figure 4.12). To carry out numerous sampling surveys to investigate reproducibility is clearly not a practical option.

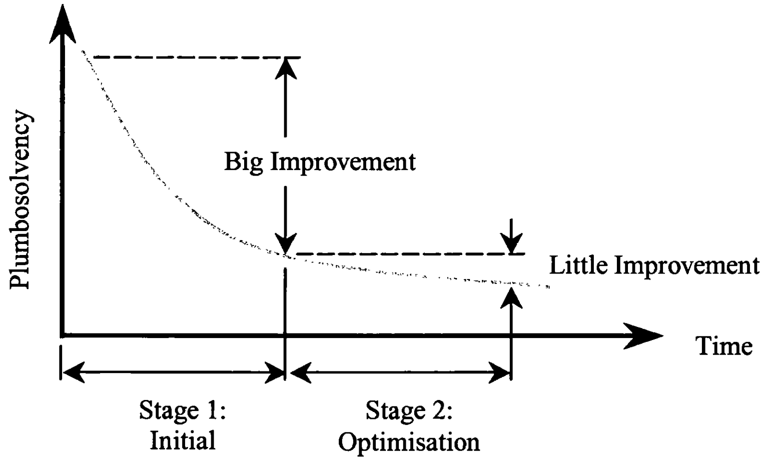


Figure 4.12. Water treatment over time.

Consequently, it is necessary to assess the random daytime sampling method, for the optimisation of plumbosolvency control using the computational model developed. The validity of the sampling method for demonstrating both the initial reductions in plumbosolvency achieved by installing corrective treatment and the subsequent reductions achieved through optimisation must be investigated. However, the issue of using random daytime sampling for assessing regulatory compliance will not be discussed.

4.2.2 Statistical testing

In order to quantify the effects of corrective water treatment on a water supply zone, e.g. orthophosphate addition, random daytime sampling is carried out both before and after treatment. Thus, we essentially have two sets of data: one set corresponding to *1-litre* sample concentrations (in *μg/l*) before treatment, and one set corresponding to *1-litre* sample concentrations (in *μg/l*) after treatment. It should be noted that the two sets of data are not paired because the house address and time of day will vary for each sample collection due to the random nature of the procedure. Therefore the two sets of data are treated as unpaired samples.

If it can be shown that, to some degree of certainty, the sample concentrations after a treatment step are lower then those before it, we may conclude that the water treatment step was successful. In other words, reject the null hypothesis H_0, where

H_0 = The samples come from the same population, i.e. the water treatment step produced no effects.

in favour of the alternate hypothesis H_1, where

H_1 = The samples originate from different populations where the mean of the population for samples taken after the treatment step is smaller than the mean of the population for samples taken before it, i.e. the water treatment step was successful.

When choosing a statistical test to use, it is necessary to observe basic properties of the data corresponding to the samples and the population from which they are taken. In the case of random daytime sampling, the populations from which samples have been taken cannot be assumed to have a normal distribution. In fact the distributions obtained from the computer model, previously described, can often be multi-modal and highly skewed, depending on the input variable distributions. It is therefore advisable to forego the *t-test* and turn instead to it's non-parametric alternative, the *Mann-Whitney test.* This test can be used in the case of unpaired samples and does not require any assumptions to be made about the population's distribution. The primary assumption of the Mann-Whitney test is that the two samples are randomly and independently drawn [75]. This non-parametric test has already been used in the field of plumbosolvency control, in particular, to quantify the effects of water treatment [59].

Since this test can be carried out on unpaired data it is possible to compare a set of n_1 values (corresponding to samples before a treatment step) with a set of n_2 values (corresponding to samples after the treatment step) where $n_1 \neq n_2$ is valid. However, the actual tests to be carried out within this investigation will have $n_1 = n_2 = n$.

The Mann-Whitney test involves assembling both sets of data into a single set, which are then ordered in rank from lowest to highest. The rankings are then returned to the sample they originally came from, then summed giving T_1 and T_2. The *U-statistic*, upon which the significance test is based, is calculated as

$$U = T_1 - \frac{n_1}{2}(n_1 + 1) \qquad \text{Eqn. 4.1}$$

A normal approximation to the distribution of *the U-statistic* can be used, and the standard normal deviate Z, from which probabilities may be calculated from, is calculated [83] as:

$$Z = \frac{U - (n_1 n_2 / 2)}{\sigma_T} \qquad \text{Eqn. 4.2}$$

where σ_T is the standard deviation of the sampling distributions for T_1 and T_2.

In most areas of scientific research, the criterion for statistical significance is conventionally set at the *5%* level [75]. Within this investigation the convention of using $P(H_0)$ to describe the value of statistical significance will be used. For convenience P will be used to represent $P(H_0)$. The following conclusions are made in these circumstances:

Table 4.12. Conclusions based on *P*.

Result	Conclusion
$P = 100\%$	samples definitely came from different populations – treatment step successful
$P > 95\%$	samples probably came from different populations – treatment step successful
$5\% < P < 95\%$	samples probably came from same population – treatment step not successful
$P < 5\%$	samples probably came from different populations – treatment step not successful
$P = 0\%$	samples definitely came from different populations – treatment step not successful

Instead of using a necessarily limited quantity of random daytime sample data obtained by actual sampling, a much more extensive range of data has been created using a numerical simulation of the random daytime sample collection process, previously described (Chapter 3.2.4.2).

The advantages of using a numerical simulation such as this is that it is able to produce vast amounts of sample data in very little time at low cost. This makes it possible to investigate the statistical significance of the effects of various degrees of water treatment for a wide range of sample sizes. Since random daytime sampling has inherent limitations, as previously discussed, the potential for considerable sample error is large, particularly when the sample sizes are small. Thus, if a second set of samples were taken before and after treatment, the statistical significance of the effects of water treatment (or P value) could be different from the first. Consequently, it is clear that the sampling procedure, and subsequently the statistical testing procedure, will have to be carried out a number, m times for each case in order to smooth out the sampling error. This will result in a distribution of values of the statistical significance (or P) from which properties such as mean and standard deviation may be calculated. Clearly, the greatest sampling error will occur when the number of samples is small; thus the standard deviation of the P values in this case will be greatest.

4.2.3 Experimental design

Water supply zones in the UK typically comprise around *10,000* properties. The proportion of properties in the UK containing lead pipework is about *40%*. To reflect these trends, the parameters of the simulated water supply zone, used in all investigations, are as follows:

Total number of properties : *10,000*
Number of properties supplied through lead pipe-work : *4,000*
The lengths of lead pipe and non-lead pipe, daily water consumption and water usage patterns all follow the standard distributions as previously described.

The plumbosolvency of the water is defined by the solubility at equilibrium E and the diffusion coefficient D for the diffusion model, or M for the exponential approximation. It is possible to simulate water treatment by controlling the D and E, or M and E parameters used in the simulation. The plumbosolvency parameters for each treatment step investigated are shown in Table 4.13. The parameters relating to *0%* treatment (untreated) are representative of a moderately plumbosolvent water such as a high alkalinity water before phosphate treatment or a low alkalinity water after pH adjustment but again before phosphate treatment.

Table 4.13. Plumbosolvency of treated water.

Treatment (Reduction in Plumbosolvency)	Plumbosolvency Parameters	
	M	E
00% (Untreated)	0.1	150
50%	0.05	75
60%	0.04	60
70%	0.03	45
80%	0.02	30
90%	0.01	15

Random daytime sampling surveys were simulated for each water treatment step a total of $m = 100$ times. This whole process was carried out for a number of different sample sizes, namely $n = 52$, *100, 200, 500, 1000, 2000,* and *5000* samples. It was intended that this range in sample numbers would provide a clearer idea of how many samples are required in order to observe the benefits of various degrees of water treatment.

The computational model has been utilized to produce output data that consists of a set of n values for each sample collection survey. The individual values correspond to the concentration (measured in $\mu g/l$) of the one-litre sample taken at a random property at a random time during the day. Note: if a sample is taken from a house that doesn't have a lead pipe, the corresponding concentration will be equal to zero. The total number of these data sets produced for this investigation and average size of data set is as follows:

Total sets of data = (no. of surveys) x (no. of treatment stages) x (no. of different sample sizes)

= 100 x 6 x 7

= 4200

Average size of data set = (52 + 100 + 200 + 500 + 1000 + 2000 + 5000) / 7 ***= 1265***

These simple calculations give an impression of the vast quantity of data that can be obtained from the software for statistical analysis. Collection of this quantity of data (over 5 million samples altogether) would not be logistically possible if it were to be carried out in the traditional manner.

Output data, produced by the sampling simulation software, is then read into a separate Mann-Whitney FORTRAN routine, which outputs corresponding values of P. Each water treatment step is compared with every other water treatment step; thus we have *15* different combinations, each is indicated by X marks (Table 4.14). Consequently *15* values were produced for every single survey for each sample size. This results in a total of *10,500* individual Mann-Whitney significance tests being carried out, and, therefore *10,500* values of *P* being produced.

Table 4.14. Combinations of treatment steps.

Comparisons		Data 2 (2nd treatment step)					
		0%	50%	60%	70%	80%	90%
Data 1 (1st treatment step)	00%		X	X	X	X	X
	50%			X	X	X	X
	60%				X	X	X
	70%					X	X
	80%						X
	90%						

4.2.4 Analysis of results

An example of the summary data obtained through multiple simulations of RDT sampling, using a sample size of *52* on a standard water supply zone is shown (Figure 4.13).

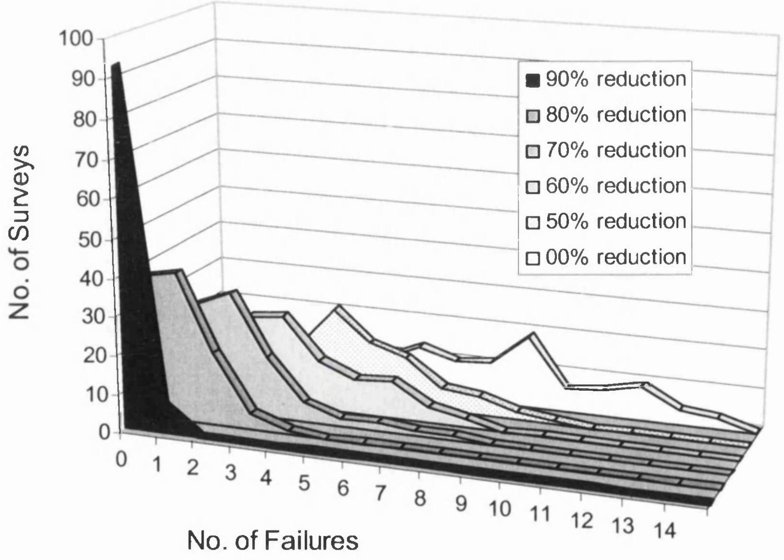


Figure 4.13. Variability in RDT failure rates.

This demonstrates the variability in failure rates occurring against the *10μg/l* standard over the *100* surveys simulated for each plumbosolvency reduction. Clearly, as the water is treated further and the plumbosolvency reduction increases, the average number of samples that fail decreases. Note that in the case of untreated water there is no clear peak in the distribution; this makes it very difficult to estimate the most likely real-world RDT failure rate.

For each sample size, output data from the Mann-Whitney solver comprises of a set of *m* values of *P* for each combination of treatment steps. The *m* values obtained for a particular case may be plotted in the form of a histogram (Figure 4.14). In this particular case the number of samples taken in each of the *m = 100* surveys was 200, and the water treatment carried out was from *00%* treated (untreated) to *50%* treated.

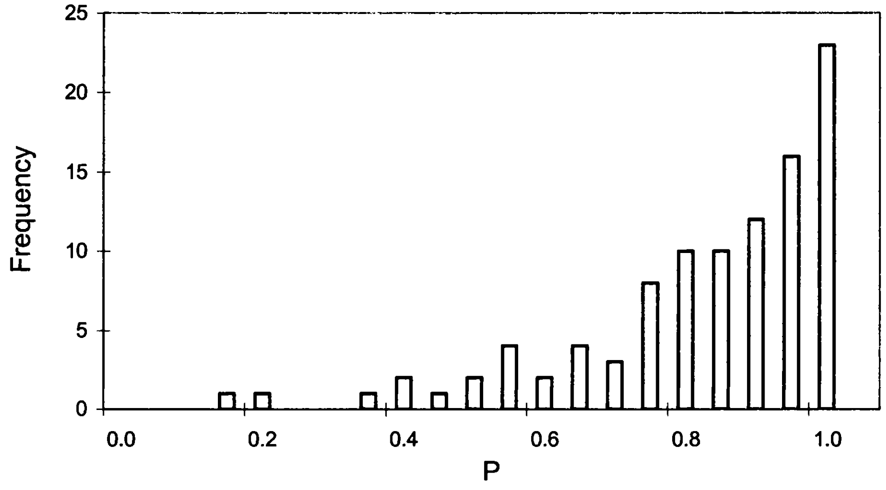


Figure 4.14. Histogram of statistical significance *P*.

These *m* values can be treated as samples from a population. The statistical parameters of the population from which these samples are taken can be estimated as follows:

$$Mean = \bar{P} = \frac{1}{m}\sum_{i=1}^{m} P_i \qquad \text{Eqn. 4.3}$$

$$StandardDeviation = \hat{\sigma} = \sqrt{\frac{m\sum_{i=1}^{m} P_i^2 - \left(\sum_{i=1}^{m} P_i\right)^2}{m(m-1)}} \qquad \text{Eqn. 4.4}$$

Note that the population estimate of the standard deviation in Eqn. 4.4 is calculated using the "nonbiased" or "*m-1*" method.

The estimated population mean, $\overline{P}$ over the 15 different combinations of treatment has been plotted for each sample size (Figure 4.15). As expected $\overline{P}$ increases with sample size, however, it is clear that there are other patterns in these data. Most notable is the rise and fall nature of $\overline{P}$ over the various combinations of water treatment. This can be explained by observing the percentage increase in the amount of water treatment, i.e. the percentage decrease in plumbosolvency between the two water steps being compared. For example, there is comparatively very little difference between *50%* treated water and *60%* treated water, thus $\overline{P}$ is consistently lower.

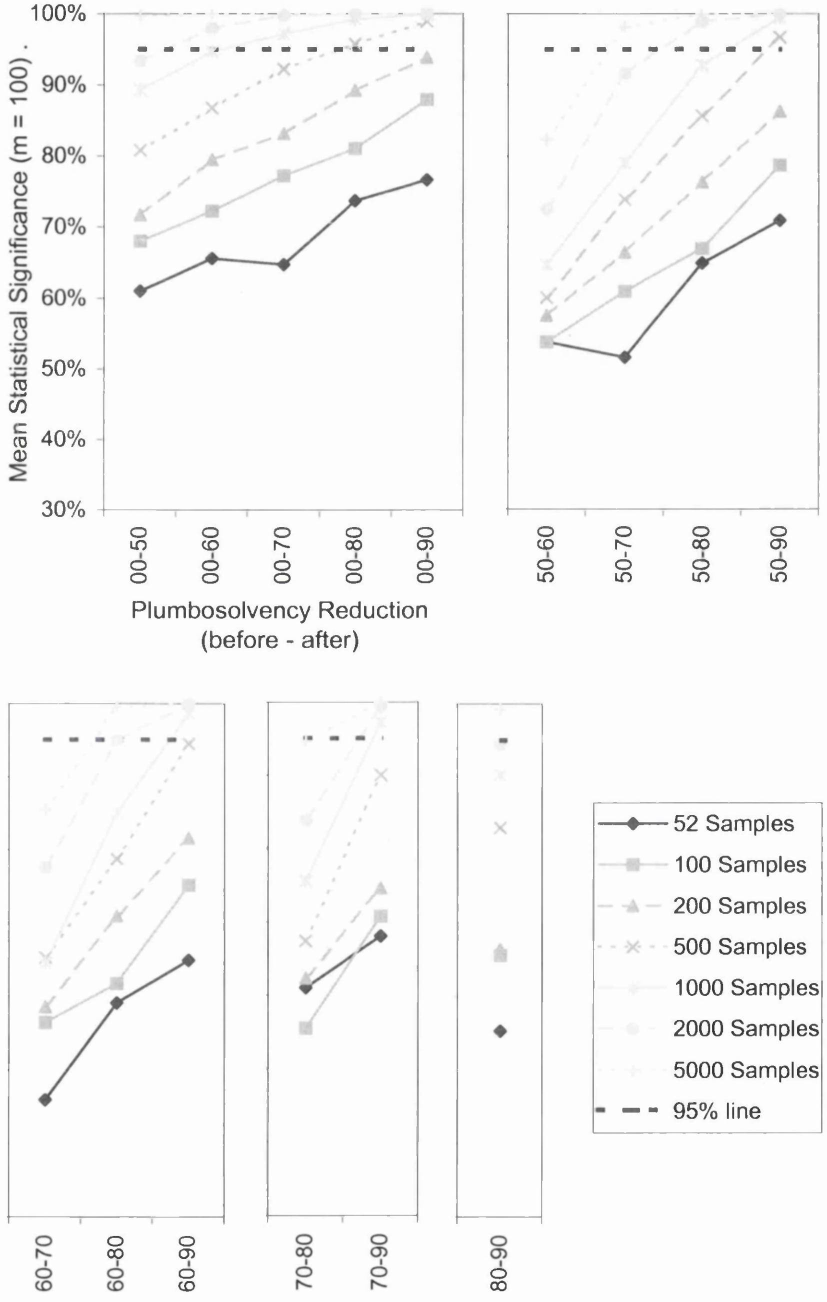


Figure 4.15. Mean statistical significance.

It is evident that there are one or two small inconsistencies within the pattern of this data. These occur where the *52 samples* line crosses the *100 samples* line, i.e. where P is higher for lower sample sizes. This is caused by sampling error, which in the case of 52 samples, has not been smoothed out completely. Clearly, increasing the number of surveys from $m = 100$ to, say, $m = 500$ should produce a more accurate *52 samples* line which follows the general pattern of the rest of the data more closely.

As previously discussed, the conclusion that the treatment produced significantly beneficial results can only be made if $P > 95\%$. Consequently, the inclusion of the *95%* line in Figure 4.15 enables one to distinguish when water treatment is significantly successful. As can be seen, a minimum of *500* samples is required in order to observe any significant benefits from water treatment; though these will only be observed in *3* of the *15* combinations of treatment. Even when *5,000* samples are taken, significant benefits will not be observed in *3* of the *15* combinations (*50-60*, *60-70*, and *70-80*). It is possible, however, to use less stringent confidence objectives. The number of samples (to be taken both pre and post treatment), n, required for observing benefit at three different levels of significance have been calculated, by interpolation, for a range of treatment scenarios (Table 4.15). It can be seen that even for the *80%* significance level, high numbers of samples continue to be required to differentiate the effects of water treatment at the optimisation stages.

Table 4.15. Sample sizes required at three different levels of significance.

Treatment Step	Significance Level 95	90	80
00-70	750	400	150
70-80	5000	3500	1500
70-90	800	500	300
80-90	2000	1000	450

For all *15* water treatment combinations (Table 4.15), the estimated population standard deviation $\hat{\sigma}$ has been plotted for each sample size (Figure 4.16). As expected, $\hat{\sigma}$ decreases with increasing sample size. This is most apparent in the cases where the level of treatment improvement is greatest, i.e. *00-90*, *50-90*, *60-90* etc. and is least apparent in the case of *50-60*. Other statistical parameters such as range can be plotted in much the same way; clearly the range of the P values would decrease as the sample size increases similarly to standard deviation.

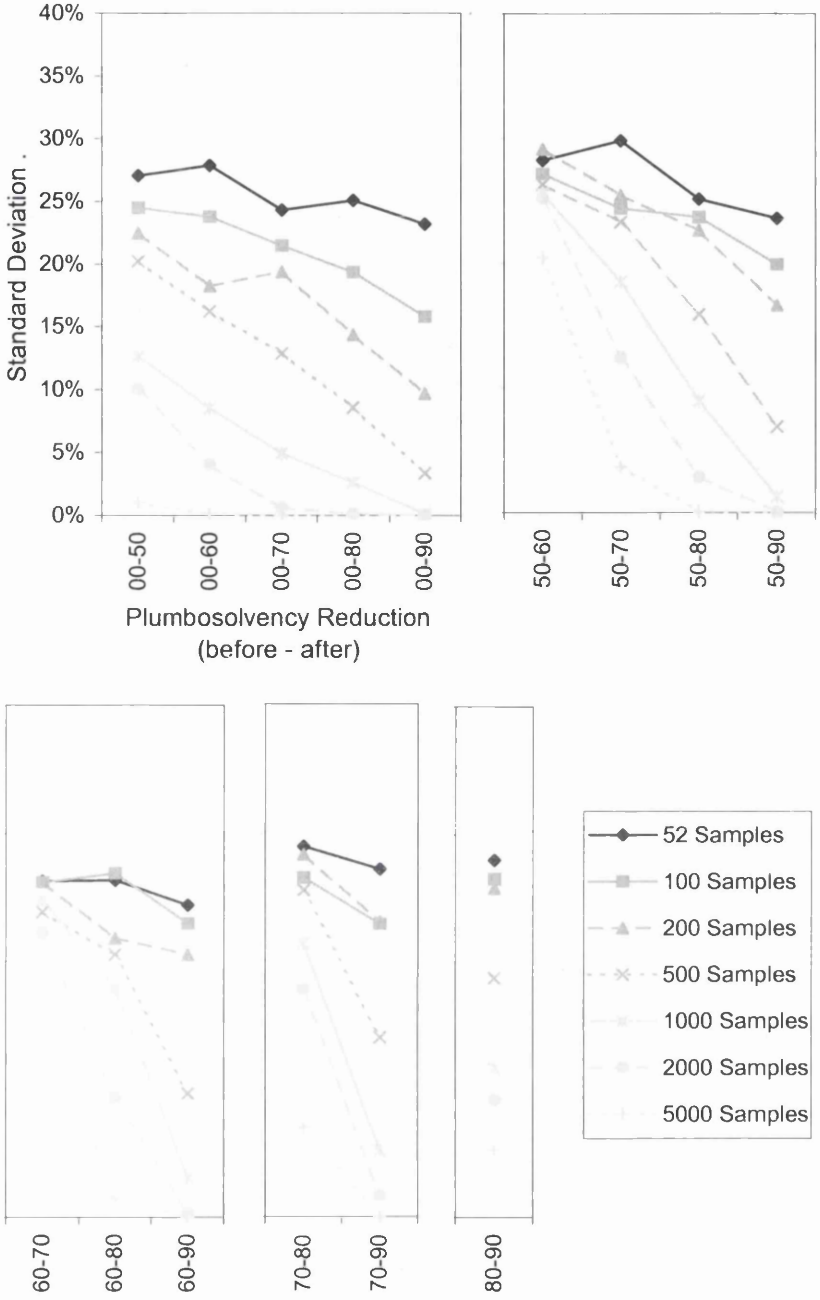


Figure 4.16. Standard deviation of statistical significances.

As well as studying the combined properties of the population, from which the samples are taken, it is also useful to observe the total number of individual surveys which show significant improvement, i.e. have a *P* value greater than *95%* (Figure 4.17).

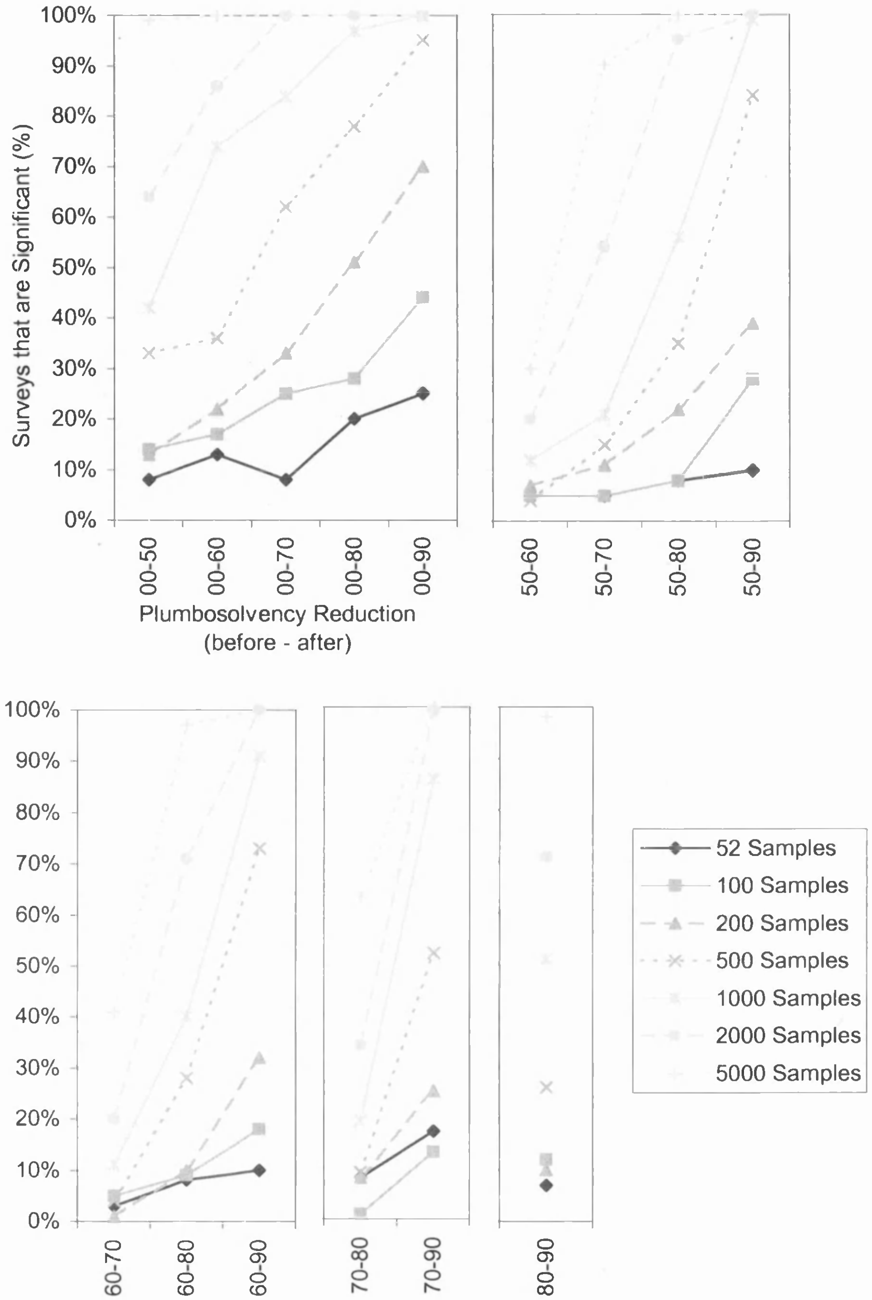


Figure 4.17. Percentage of surveys that are significant.

Figure 4.17 clearly demonstrates how a very low proportion of the surveys showed significant improvement in the case of comparing *50%* treatment with *60%* treatment, even for very large sample sizes. Although $\overline{P}$ in the case of *5,000* samples is over *80%* (Figure 4.15), a mere *30* out of the *100* surveys were actually over *95%* thus making them statistically significant. This would indicate that somewhere in the region of *10,000* samples would need to be taken, both pre and post treatment, in order to have a

50-50 chance of observing a significant benefit when going from *50%* to *60%* treatment.

Once again, there are clearly patterns in the data, such as the rises and falls, as well as small inconsistencies, particularly in the case of small sample sizes. These correspond to the patterns and inconsistencies found in Figure 4.15 and can be explained in exactly the same way.

4.2.5 Discussion and conclusions

Results from the Mann-Whitney tests show that the chance of observing statistically significant beneficial effects from water treatment increases with sample size. However, beneficial effects were not observed for *3* of the *15* water treatment steps (*50-60*, *60-70*, and *70-80*) when testing at the *95%* level of significance, even when *5,000* samples were taken. Additionally, by repeating each sample collection and significance test many times it has been possible to observe the likely spread of results, i.e. standard deviation of the significance values *P*. As expected, the standard deviation decreases with increasing sample size. This has been most apparent in the cases where the level of treatment improvement is greatest, i.e. *00-90*, *50-90*, *60-90* etc. The operational significance of such sampling error is that water managers may be misled by the laws of chance that are inherent in such a sampling technique.

It has also been shown that somewhere in the region of *10,000* samples would need to be taken, both pre and post treatment, in order to have a *50-50* chance of observing benefit at the *95%* level of significance, when going from a *50%* to a *60%* treatment level. Smaller sample sizes are required if the confidence level is lower; however, they are still too large for practical consideration in cases where it is intended to differentiate the effects of water treatment at the optimisation stages. Thus, for the quantification of the effects of treatment optimisation, particularly where the extent of treatment change is small, the random daytime sampling procedure is not suitable. A similar conclusion has been made by Cardew [59] from the comparisons of RDT results before and after the installation of phosphate dosing across much of the NW of England. Cardew quotes "circa *16,000*" measurements per annum as the number required to differentiate a *25* to *30%* seasonal difference in lead results, however this relates to the region not individual water supply zones.

This statistical analysis of computer simulated data clearly confirms that the UK's Drinking Water Inspectorate is correct in being concerned at the possible use by water companies of random daytime sampling for the optimisation of plumbosolvency treatment measures, particularly for individual water supply zones or small clusters of zones that have similar water quality characteristics.

4.2.6 Summary

In order to quantify the effectiveness of corrective water treatment for plumbosolvency control, compliance samples, in respect of the lead parameter, must be taken from the point of use by consumers. The favoured sampling method is RDT, however, it is believed [22,48] that random daytime sampling is insufficiently reproducible. Consequently, the random daytime sampling method has been assessed for the optimisation of plumbosolvency control using the computational model developed.

Extensive sample data has been created using the computational model, which is able to simulate the process of random daytime sampling for varying levels of water treatment. The advantages of using a numerical simulation, as opposed to actual data collection, is its ability to produce vast amounts of sample data in very little time at low cost. Consequently it is possible to simulate multiple RDT sampling surveys and investigate reproducibility of RDT sampling.

The analysis of the simulated sample data has been carried out using a non-parametric statistical test for unpaired samples, the Mann-Whitney U-test. Using this test it has been possible to compute the probability of whether, overall, the sample concentrations after a treatment step are lower than those before a treatment step. A number of different treatment steps were studied and a range of sample sizes was investigated.

It has been found that for the quantification of the effects of treatment optimisation, particularly where the extent of treatment change is small, the random daytime sampling procedure is unsuitable.

5 CONCLUSIONS

5.1 Introduction

At the time of writing, the issue of lead in drinking water is highly pertinent to water supply companies within the U.K, as the standard for lead in drinking water will be tightened from 50µg/l to 25µg/l in December 2003. However, the issue will be of major concern for a further 10 years, as the standard will tighten to 10µg/l in December 2013 in light of the justified health concerns.

Until recently, the only approach for achieving the new lead standards had been widely considered to be the replacement of lead pipes with piping of an alternative non-toxic material. However, the potential success of corrective water treatment, in the form of phosphate dosing at the correct pH, has now become better appreciated, particularly as a result of the experience of many UK water authorities and companies.

In order to optimise corrective treatment, accurate monitoring of lead emissions across a water supply zone must be achieved. However, traditional monitoring methods, such as Random Daytime sampling, are deemed to be inadequate because lead emissions are highly variable at individual houses, a problem that is compounded across a water supply zone. This has justified the development of additional techniques such as computer simulation. However, to date, the majority of such techniques have been of limited use since they do not provide the flexibility to investigate lead emissions at a single house as well as zonal treatment strategies. The limitations of existing computational models have provided the motivation to develop a more complete model for use, by water engineers, to assess compliance, and facilitate the optimisation of corrective treatment as well as to investigate lead emissions at individual houses.

5.2 Single house

The development of a model to assess lead in drinking water, described within this thesis, has been achieved primarily by considering the factors that influence lead emissions at a single house as well as across a water supply zone and applying the mathematics that describe the physical processes taking place within the pipework. The complete model is broken into two main components, the single house model and the zonal model.

The single house model comprises a number of increasingly sophisticated modelling options for pipe flow and mass transfer. Two models have been investigated to simulate the transfer of lead into the water within a pipe. An analytical solution as well as a numerical solution has been developed for the more complex diffusion model. These models have also been substantiated by experimental results, which have allowed the diffusion models to be calibrated more fully. Three models have been investigated to simulate the flow of water through a pipe. These flow models have been used in conjunction with the equation of mass transfer to simulate the concentration of lead at the tap. Thus, it has been possible to model instantaneous concentrations more realistically and in more detail than previously achieved. This has enabled the various flow and mass transfer options to be investigated for a number of individual situations, including flow periods and stagnation periods. The results illustrate how lead emissions vary within the pipe over time during stagnation and flow.

By applying a pattern of water usage, the daily variation of lead emissions has been investigated and an 'average' concentration, consistent with the way in which the new EU lead standards are specified in the Directive, has been computed. The computation of the daily average concentration of lead has allowed the factors that influence lead emissions at a single house to be investigated for the purposes of understanding the general issues that relate to plumbosolvency control. This has revealed that the major factors influencing lead emissions, in terms of daily average concentration, are:

- Plumbosolvency of the water; the average concentration of lead emissions increases in direct proportion to increases in factors M and E (exponential model) and factors D and E (diffusion model).
- Length of lead pipe; the average concentration of lead emissions increases in direct proportion to length up to about 100m.
- Volume of water used in the day; the average concentration of lead emissions increases exponentially as the volume decreases.
- Diameter of pipework; the daily average lead concentration increases as the diameter of the lead pipe increases.

- Frequency of water use; daily average lead emissions increase with frequency of water use for a given daily volume, the effect is only significant in the case of the diffusion model.

Less important influencing factors are:

- Flow rate; daily average lead emissions are slightly higher at lower flow rates.
- Pattern of water use; whilst the contact time of the water in the lead pipe very much determines the instantaneous concentrations of lead, the effects are much less important in determining the average lead concentration.

In addition to daily average concentration, the standard "30-minute stagnation" test, widely used in the UK for benchmarking the success of plumbosolvency control treatment, has also been modelled by applying an appropriate water usage pattern. Results indicate that 30-minute stagnation sample concentration decreases rapidly with increasing length of non-lead pipe between the lead pipe and the point of emission. Consequently, the method is deemed unsuitable for survey purposes in assessing zonal compliance, since houses selected at random will have different lengths of non-lead pipe-work.

5.3 Water supply zones

The primary objective of this research, from a zonal perspective, was to develop a computational model, to be used by water engineers, to assess zonal compliance and facilitate the optimisation of corrective treatment. This has been achieved by integrating the single house model into a Monte Carlo probabilistic framework in order to describe the wide variation of influencing factors that occurs across a water supply zone. Integration of the single house model has also facilitated subsequent modifications and provides a more convenient 'all in one' solution.

By use of a Monte Carlo approach, a complete zone can be described in great detail and a number of different monitoring methods, including Random Day Time (RDT) sampling can be simulated. A detailed description of the simulated water supply zone has allowed greater understanding of the likely characteristics of problem houses, where lead emissions are highest. Other advantages of the zonal model that has been developed include:

- Specification of zonal circumstances is highly flexible to facilitate best possible calibration to local circumstances.
- Capability to save, load and alter detailed descriptions relating to complete water supply zones.

- Capability to handle complex branched systems of pipework.
- Average lead emission concentrations can be simulated, consistent with the way in which the new EU lead standards are specified in the Directive.
- A range of sampling techniques can be evaluated in much more detail, including their reproducibility.

The results of simulated RDT sampling from the zonal model have been validated for a wide range of real water supply zones by reference to RDT sample results from the water companies, enabling the model to be used confidently for predictive purposes. Analysis of results from both zonal and single house simulations has revealed that the more simplistic yet computationally much faster plug flow – exponential model is an adequate approximation to the more realistic turbulent – diffusion model and can therefore be confidently employed for routine zonal simulations. This satisfies a primary aim of this research, namely to develop a computational model that can run on modest computing resources.

Zonal case studies have been completed satisfactorily for a wide range of real water supply zones, establishing the percentage reduction in plumbosolvency required to achieve compliance targets to be determined. This has facilitated a simple system of quality control which can be based on fixed point monitoring, the approach to monitoring preferred by the DWI. For the 'South England' example case study, included in this thesis, it has been concluded that:

- The 25 μg/l standard for lead should be readily achieved by optimised phosphate dosing (at the correct pH), without having to replace lead pipes, unless the water has a high organic loading or is significantly discoloured by iron.
- Realistic treatment targets for plumbosolvency reductions of between 60 and 85% will minimise non-compliance with the 10 μg/l standard for lead to a sufficient extent that will permit any lead pipe replacement to be selective and greatly minimised.
- The case study undertaken suggests that the treatment targets for plumbosolvency reduction could be, as a guide to optimisation: (a) <1.5% zonal failure based on average lead concentrations, (b) <4.0% RDT failure, and (c) <200 houses require further attention, expected to be part or total replacement of their lead pipes.
- The identification of such remaining problem houses should be feasible from the knowledge of the minimum lengths of lead piping involved in conjunction with residency. As a general guide, cases studies undertaken using the model indicates that the minimum length of lead pipe will be about 30 to 40m, which should be fairly easy to find.

The facility of the model to simulate repeated RDT sampling surveys has demonstrated the lack of reproducibility in such sampling and also enabled a detailed assessment of the use of this monitoring method for the optimisation of plumbosolvency control. This assessment has been carried out using a non-parametric statistical test for unpaired samples, the Mann-Whitney U-test. Results conclude that the RDT sampling procedure is unsuitable for the quantification of the effects of treatment optimisation, particularly where the extent of treatment change is small. This has confirmed that the UK's Drinking Water Inspectorate is correct in being concerned at the possible use by water companies of random daytime sampling for the optimisation of plumbosolvency treatment measures, particularly for individual water supply zones or small clusters of zones that have similar water quality characteristics.

5.4 Future work

Sufficient progress in computational modelling has now been made to provide water engineers with a further powerful tool for achieving the cost effective rectification of plumbosolvency problems in their water supplies. However, it should always be recognised that results from the model, particularly those relating to zonal compliance, are approximations and not true values. This is because even the most sophisticated modelling options in the single house model are simplifications of the numerous complex chemical and physical processes occurring at a single house. Additionally, in the case of water supply zones, parameters such as the distribution of pipework lengths are rarely precisely known and must be estimated.

There is little that can be done to improve the accuracy of the parameters used in the zonal model aside from obtaining more comprehensive survey data from the water supply zone being modelled, a task that rests on the water supply company. However, the accuracy of results from both the single house and zonal models can be increased by developing a more accurate model for the flow and mass transfer processes as well as considering additional factors that may influence lead emissions.

While the accuracy of the diffusion model cannot significantly be improved without further experimental evidence, there is scope to improve the accuracy of the exponential approximation. This may be achieved by using a modified log-hyperbolic function to resemble the diffusion curve more closely. Such a function would require additional parameters, the values of which would be dependant on diameter of pipework. Although this would be relatively easy to implement, it should be noted that the solution would still not model the radial variation of lead in the pipe.

There is certainly scope to develop a more accurate description of the flow regime within the pipework, possibly using a full finite volume solution. This would allow a more accurate description of instantaneous lead emissions and would be able to take into account the bends and curves in the plumbing. Additionally, the effects of flow events such as the water-hammer effect may also be studied on a number of different pipe systems using such a solution. This work would be useful in studying the influence of specific pipework configurations and flow events on lead emissions. However, it would not be feasible to apply such a model to a complete water supply zone since the run time required would be far too great for routine calculations.

Particulate lead has been suggested as one of the primary causes of extremely high lead levels, occasionally found in drinking water and is thought to be caused by the flaking of fragile lead corrosion products from the inside wall of the lead pipe. While it is possible to estimate the shear forces on the pipe wall, it is not known how this relates to the amount of lead that is flaked off the pipe surface. However, there are a number of alternative methods that could be investigated for the purposes of accounting for the occurrence of particulate lead. A possible solution might involve applying a distribution that describes the probability and magnitude of particulate lead across a zone using a Monte Carlo method, in a similar way to pipework lengths. However, actual survey data will be required in order to estimate the possible occurrence and extent of particulate lead.

In addition to accuracy, there is scope to improve the run time of the model without sacrificing accuracy and functionality, in particular to increase the speed of routine zonal simulations. This has already been carried out to some extent by optimising the discretisation used within the model for the required purposes, based on an analysis of the effect of discretisation. However, additional model parameters and routines will need to be investigated more fully to determine where further optimisations may be achieved.

6 BIBLIOGRAPHY

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[1] ENCYCLOPÆDIA BRITANNICA INC, [2002, Encyclopædia Britannica Premium Service WWW]. http://www.britannica.com/eb/, June 2002.

[2] MICROSOFT CORPORATION, [2002, Encarta Online Encyclopaedia WWW]. http://encarta.msn.com, June 2003.

[3] AINSWORTH, R.G., BAILEY, R.J., COMMINS, B.T., PACKHAM, R.F. & WILSON, A.L. 1977. Lead in Drinking Water: Considerations relating to proposed new limit of 0.05 mg/l. *Water Research Centre*, Technical Report TR 43.

[4] LEWIS, J., [1985, Lead Poisoning: A Historical Perspective. EPA History Office WWW]. http://www.epa.gov/history/, June 2002.

[5] DALE DORMAN LTD. [1994, Your Drinking Water: Lead, Circular 819 WWW]. http://www.ces.uga.edu, June 2002.

[6] CHUDLER E.H., [2001, Get the Lead Out! The Effects of Lead on the Nervous System. Neuroscience for Kids WWW]. http://faculty.washington.edu/chudler/, June 2002.

[7] SCHOCK, M.R., WAGNER, L. & OLIPHANT R.J. 1996. Corrosion and Solubility of Lead in Drinking Water. *In :* AWWA. 2nd ed., *Internal Corrosion of Water Distribution Systems*. Denver, CO., pp.131-230.

[8] BACON, A.P.C., FROOME, K., GENT, A.E., COOKE, T.K. & SOWERBY, P. 1967. Lead Poisoning from drinking soft water, *The Lancet*, **7484** (1), pp.264-266.

[9] BEATTIE, A.D., DAGG, J.H., GOLDBERG, A. & WANG, I. 1972. Lead poisoning in rural Scotland. *British Medical Journal*, **812** (2), pp.488-491.

[10] BEATTIE, A.D., MOORE, M.R., DEVENAY, W.T., MILLER, A.R. & GOLDBERG, A. 1972. Environmental lead pollution in an urban soft water area. *British Medical Journal*, **313** (2), pp.491-493.

[11] WATT, G.C.M., BRITTON, A., GILMOUR, W.H., MOORE, M.R., MURRAY, G.D., ROBERTSON, S.J. & WOMERSLEY, J. 1996. Is lead in tap water still a public health problem? : An observational study in Glasgow. *British Medical Journal,* **313** (2), pp.979-981.

[12] MACDONELL, J.E., CAMPBELL, H. & STONE, D.H. 2000. Lead levels in domestic water supplies and neural tube defects in Glasgow. *Archives of Disease in Childhood*, **82** (1), pp.50-53.

[13] LACEY, R.F., MOORE, M.R., RICHARDS, W.N. 1985. Lead in water, infant diet and blood: the Glasgow Duplicate Diet Study. *The Science of the Total Environment*, **41** (3), pp.235-257.

[14] SHERLOCK, J.C., QUINN, M.J. 1986. Relationship between blood lead concentrations and dietary lead intake in infants: the Glasgow Duplicate Diet Study 1979-1980. *Food Additives and Contaminants*, **3** (2), pp.167-176.

[15] MACINTYRE, C., FULTON, M., HEPBURN, W., YANG, S.Y., RABB, G., DAVIS, S., HEAP, M., HALLS, D. & FELL, G. 1998. Changes in blood lead and water lead in Edinburgh. An eight year follow-up to the Edinburgh lead study. *Environmental Geochemistry and Health*, **20** (3), pp.157-167.

[16] KARHAUSEN, L. 1973. Intestinal lead absorption. *In* : *International symposium on environmental health aspects of lead, Amsterdam, 1972.* Luxembourg, C.E.C., pp.427-440.

[17] SPECTRUM LABORATORIES INC, [2002, Chemical Fact Sheet (Lead) WWW]. http://www.speclab.com/elements/lead.htm, June 2002.

[18] NATURAL SOLUTIONS ENVIRONMENTAL, INC, [1999, Lead in drinking water WWW]. http://www.naturalsolutions1.com/lead.htm, June 2002.

[19] NORTH WEST WATER LTD, [1999, Background Briefing on Lead WWW]. http://www.nww.co.uk, June 2002.

[20] PACKHAM, R.F. 1971. The leaching of toxic substances from unplasticized PVC water pipe. *Water Treatment and Examination*, **20**, pp.144-164.

[21] HAYES, C.R. 2002. Environmental Water Management: Lead in drinking water Lecture Notes. Department of Civil Engineering, University of Wales, Swansea.

[22] VAN DEN HOVEN, T.J.J., BUIJS, P.J., JACKSON, P.J., MILLER, S., GARDNER, M., LEROY, P., BARON, J., BOIREAU, A., CORDONNIER, J., WAGNER, I., MARECOS DO MONTE, H., BENOLIEL, M.J., PAPADOPOLOUS, I. & QUEVAUVILLER, P. 1999. Developing a new protocol for the monitoring of lead in drinking water. European Commission Report EUR 19087, ISBN 92-828-6888-5.

[23] BRYCE-SMITH, D. 1989. Health considerations - is there a need for tighter water-lead standards? *In : IWEM Symposium on Lead in Water. London, April 1989.*

[24] CHAMBERS, K. & HITCHMOUGH, M. 1992. Economics of lead pipe replacement. Report DoE 2956-/1, TMU 9030. London: House of Commons Library.

[25] THE STATIONERY OFFICE LTD. 2000. The Water Supply (Water Quality) Regulations 2000, Statutory Instrument 2000 No. 3184.

[26] WORLD HEALTH ORGANISATION. 1993. Guidelines for drinking water quality. Volume 1, Recommendations. Geneva.

[27] WORLD HEALTH ORGANISATION. 1958. International standards for drinking water. 1st ed. Geneva, The Organization, 1971.

[28] WORLD HEALTH ORGANISATION. 1961. European standards for drinking water. 1st ed. Geneva, The Organization, 1961.

[29] EUROPEAN COMMISSION. 1980. Council Directive (80/778/EC) of 15 July 1980 relating to the quality of water intended for human consumption. Official Journal, L229 (23), 30 August 1980.

[30] EUROPEAN COMMISSION. 1998. Council Directive (98/83/EC) of 3 November 1998 on the quality of water intended for human consumption. Official Journal, L330 (32), 5 December 1998.

[31] U.S. ENVIRONMENTAL PROTECTION AGENCY. 2000. National Primary Drinking Water Regulations for Lead and Copper; Final Rule. Federal Register, **65** (8): Rules and Regulations. January 12, 2000.

[32] DRINKING WATER INSPECTORATE. 2000. Determination of requirements to meet new lead standards. Information Letter 12/2000.

[33] DRINKING WATER INSPECTORATE. 2001. Further guidance on requirements to meet new lead standards. Information Letter 3/2001.

[34] HAYES, C.R., CROLL, B.T., ELPHICK, A., VAN DER LEER, D. & WEATHERILL, N.P. 2003. Lead in drinking water: coming to terms with the new EU standards and the options for achieving optimum compliance. *J. CIWEM* (submitted).

[35] HAYES, C. R. 2000. Determining the extent to which the lead problem can be resolved by treatment rather than replacement. *IIR Annual Industry Forum on Mains Rehabilitation, London, 11th April 2000.*

[36] Boyd, G.R., Tarbet, N.K., Oliphant, R.J., Kirmeyer, G.J., Murphy, B.M. & Serpente, R.F. 2000. Lead pipe rehabilitation and replacement techniques for drinking water service - survey of utilities. *Tunnelling and Underground Space Technology*, **15** (1), pp.59-63.

[37] Boyd, G.R., Tarbet, N.K., Oliphant, R.J., Kirmeyer, G.J., Murphy, B.M. & Serpente, R.F. 2000. Lead pipe rehabilitation and replacement techniques for drinking water service: review of available and emerging technologies. *Tunnelling and Underground Space Technology*, **15** (1), pp.13-24.

[38] Colling, J.H., Croll, B.T., Whincup, P.A.E. & Harward, C. 1992. Plumbosolvency effects and control in hard waters. *J. IWEM*, **6**, pp.259-269.

[39] Sheiham, I. & Jackson, P.J. 1981. The scientific basis for control of lead in drinking water by water treatment. *J. Institution of Water Engineers and Scientists*, **35** (6), pp.491-515.

[40] Department of the Environment. 1984. Report of the Expert Advisory Group on Remedial Water Treatment for Reducing Lead Concentrations in Tap Water. Lead in Potable Water. Technical Note No. 5, (official use only).

[41] Gregory, R. & Jackson, P.J. 1983. Reducing lead in drinking water, pH adjustment and ortho-phosphate dosing to reduce lead solubility. *In :* Water Research Centre. *Regional Seminars, May 1983*. 219-S.

[42] Boffardi, B.P. 1990. Minimisation of lead corrosion in drinking water. *Environmental Treatment and Control*, **29** (8), pp.45-49.

[43] Colling, J.H., Whincup, P.A.E. & Hayes, C.R. 1987. The measurement of plumbosolvency propensity to guide the control of lead in tapwaters. *J. IWEM*, **1** (3), pp.263-269.

[44] Markall, R. 2001. Experiences in the plumbosolvency control of hard waters and expectations for complying with the new lead standards. *In : Proceedings of "Getting to Grips with Lead: A Technical Seminar on Lead in Drinking Water", London, December 2000*. CIWEM.

[45] Hayes, C.R., Bates, A.J., Goodman, A.H., Vinson, J.P. & Sadler, T.P. 1997. Meeting standards for lead in drinking water. *J. CIWEM*, **11**, pp.257-263.

[46] Croll, B.T. 2001. Applying science to the optimisation of plumbosolvency control. *In : Proceedings of "Getting to Grips with Lead: A Technical Seminar on Lead in Drinking Water", London, December 2000*. CIWEM.

[47] Jackson, P. 2001. Monitoring the Performance of Corrective Treatment Methods. *In : Proceedings of "Getting to Grips with Lead: A Technical Seminar on Lead in Drinking Water", London, December 2000*. CIWEM.

[48] CIWEM. 2001. Notes on discussion. *In : Proceedings of "Getting to Grips with Lead: A Technical Seminar on Lead in Drinking Water", London, December 2000*. CIWEM.

[49] Bailey, R.J. & Russell, P.F. 1981. Predicting drinking water lead levels. *Environmental Technology Letters*, **2**, pp.57-66.

[50] Kuch, A. & Wagner, I. 1983. A mass transfer model to describe lead concentrations in drinking water. *Water Research*, **17** (10), pp.1303-1307.

[51] van den Hoven, T.J.J. 1987. A new method to determine and control lead levels in tap water. *Aqua*, **6**, pp.315-322.

[52] Clement, M., Seux, R. & Rabarot, S. 2000. A practical model for estimating total lead intake from drinking water. *Water Research*, **34** (5), pp.1533-1542.

[53] Cardew, P.T. 2000. Simulation of lead compliance data. *Water Research*, **34** (8), pp.2241-2252.

[54] Hayes, C.R., Weatherill, N.P. & Sharp, R.J. 1999. Computer Simulation of lead emissions across an entire water supply zone (Technical Note). *In : CIWEM Workshop, London, March 1999.*

[55] Jackson, P.J. & Sheiham I. 1980. Calculation of lead solubility in water. *Water Research Centre*, Technical Report TR 152.

[56] SCHOCK, M.R. 1980. Response of lead solubility to dissolved carbonate in drinking water. *J. AWWA*, **72** (12), pp.695-704.

[57] SCHOCK, M.R. 1980. Computer Modelling of Solid Solubilities as a Guide to Treatment Techniques. *In : Seminar for Corrosion Control in Water Distribution Systems, Cincinnati, USA, May 1980.* U.S. EPA.

[58] GREGORY, R. 2000. The impact of organics on lead release. *In : AWWA International Distribution System Research Symposium, Denver, USA, June 2000.*

[59] CARDEW, P.T. 2000. Experience in the plumbosolvency control of soft waters and expectations for complying with the new lead standards. *In : Proceedings of "Getting to Grips with Lead: A Technical Seminar on Lead in Drinking Water", London, December 2000.* CIWEM.

[60] WATER QUALITY MANAGEMENT LTD. 1999. Results from plumbosolvency testing.

[61] WATER QUALITY MANAGEMENT LTD. 1999 - 2002. Private Communication.

[62] BAILEY, R.J., JOLLY, P.K., LACEY, R.F. 1986. Domestic Water Use Patterns. *Water Research Centre*, Technical Report TR 225.

[63] BUCHBERGER, S.G. & WELLS, G.J. 1996. Intensity, duration, and frequency of residential water demands. *ASCE Journal of Water Resources Planning and Management*, **122** (1), pp.11-19.

[64] BOWEN, P.T., HARP, J.F., BAXTER, J.W. & SHULL, R.D. 1993. Residential Water Use Patterns. *AWWA Research Foundation*, Denver, USA.

[65] BUCHBERGER, S.G. & WU, L. 1995. Model for instantaneous residential water demands. *J. Hydraulic Engineering, ASCE*, **121** (3), pp.232-246.

[66] DANIELSON, L.E. 1979. An analysis of residential demand for water using micro time-series data. J. *Water Resources Research*, **15** (4), pp.763-767.

[67] VEWIN. 1987. Advice for the approach to the problem of lead in drinking water (in Dutch).

[68] WS ATKINS CONSULTANTS LTD. 2001. DWI / OFWAT Joint Serviceability Study, Performance Analysis, Phase 2 Report – Rev. 1. 3rd May, 2001.

[69] CRANK, J. 1975. The Mathematics of Diffusion. Oxford, Clarendon Press.

[70] CHADWICK, A. & MORFET, J. 1993. Hydraulics in Civil and Environmental Engineering. 2nd ed. London, E & FN Spon.

[71] WEISSTEIN, E.W., [2002, Eric Weisstein's world of Physics WWW]. http://scienceworld.wolfram.com/physics/, June 2002.

[72] VAN DER LEER, D., WEATHERILL, N.P., SHARP, R.J. & HAYES, C.R. 2002. Modelling the diffusion of lead into drinking water. *Applied Mathematical Modelling*, **26** (6), pp.681-699.

[73] WATSON, G.N. 1944. A Treatise on the Theory of Bessel Functions. 2nd ed. Cambridge, University Press.

[74] HAYES, C.R. 2000. Design and Operating Protocol for Lead Pipe Test Rig. Private Communication.

[75] LOWRY, R., [1999, Concepts and Applications of Inferential Statistics WWW]. http://faculty.vassar.edu/~lowry/webtext.html, January 2001.

[76] WEATHERILL, N.P. 1997. Environmental Water Management: Mathematical Modelling Lecture Notes. Department of Civil Engineering, University of Wales, Swansea.

[77] COMPUTATIONAL SCIENCE EDUCATION PROJECT, [1995, Introduction to Monte Carlo Methods WWW]. http://csep1.phy.ornl.gov/mc/mc.html, June 2002.

[78] ORLOB, G.T. 1983. Mathematical Modelling of Water Quality. New York, Wiley Interscience Publishers.

[79] WARN, A.E. & BREW, J.S. 1980. Mass Balance. *Water Research*, **14**, pp.1427-1434.

[80] BATES, A., CUTHILL, A., JONES, L. & HAYES, C.R. 2002. Summary of case studies using a computational model in Bristol Water, Cambridge Water and South West Water. *In :* DWI-UKWIR. *Seminar on the optimisation of plumbosolvency control, 30th May 2002.*

[81] HAYES, C.R. 2002. PhD thesis: Simulation of lead emissions to drinking water – the development and application of computational methods for optimising plumbosolvency control. University of Wales Swansea.

[82] WATER QUALITY MANAGEMENT LTD. 2002. Zonal modelling of water supplies in a Portuguese City for optimisation of plumbosolvency control. Commercially confidential.

[83] COOKE, D., CRAVEN, A.H. & CLARKE, G.M. 1982. Basic Statistical Computing. London, Edward Arnold Ltd.

day. In fact, on close inspection, it is apparent that the duration of the actual peak concentrations is smaller and that the steady-state concentration is never fully achieved. This is a direct result of the significant boundary layer thickness found in laminar flow as previously discussed.

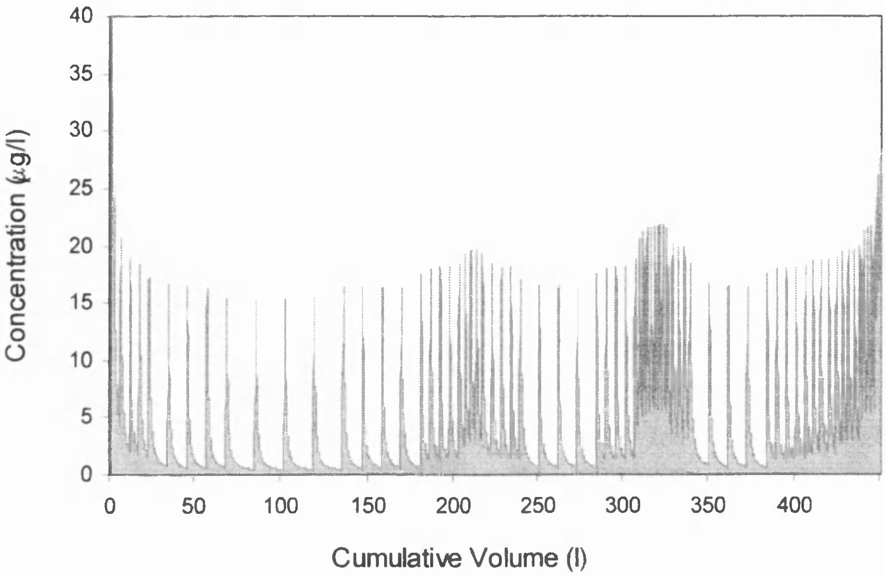

Figure 2.28. Daily concentration variation (10m lead) using laminar flow.

The solution (Figure 2.28) also illustrates how the concentration becomes elevated at several points in the day as the troughs become less well defined. This compounded effect is produced when the flow periods are of insufficient length to completely draw the lead saturated water through the tap. Consequently, high concentrations of lead will remain in the water standing within the lead and copper pipework at the start of the stagnation period. The subsequent stagnation period will thus elevate concentrations further.

The compound effect can be illustrated more clearly by the solution obtained using the plug flow - exponential model for *50m* lead pipework as opposed to *10m* lead pipework (Figure 2.29). In this case, the lead saturated water can only be flushed from the pipework if the flow period is greater than approximately one minute. Consequently, when flow periods are smaller than one minute, a compounded effect is produced. A standard compound effect is witnessed after approximately *100l* of water has been drawn; the subsequent peaks of *50μg/l* represent water that had been standing in the lead pipework for two separate stagnation periods. Similarly, peaks at *68μg/l* and *83μg/l* represent water that had been standing in the lead pipework for three and four separate stagnation periods, respectively.

4.1.6.4 Configuration of zone

As previously discussed, the water supply zone is assumed to comprise of three different types of dwellings, namely single dwellings, flats in small blocks and flats in large blocks. By observing the total consumptions for each type of dwelling (Figure 4.7), it is clear that approximately one third of all dwellings within the zone are single dwellings, one third are flats in small blocks and one third are flats within large blocks. Again, this is a reasonable assumption considering the zone is within a large provincial city.

For simplicity, it is assumed that small blocks comprise one floor having *3* flats and large blocks comprise two floors having *3* flats on each floor. The resulting configuration of the zone in terms of connectivity is illustrated (Figure 4.9).

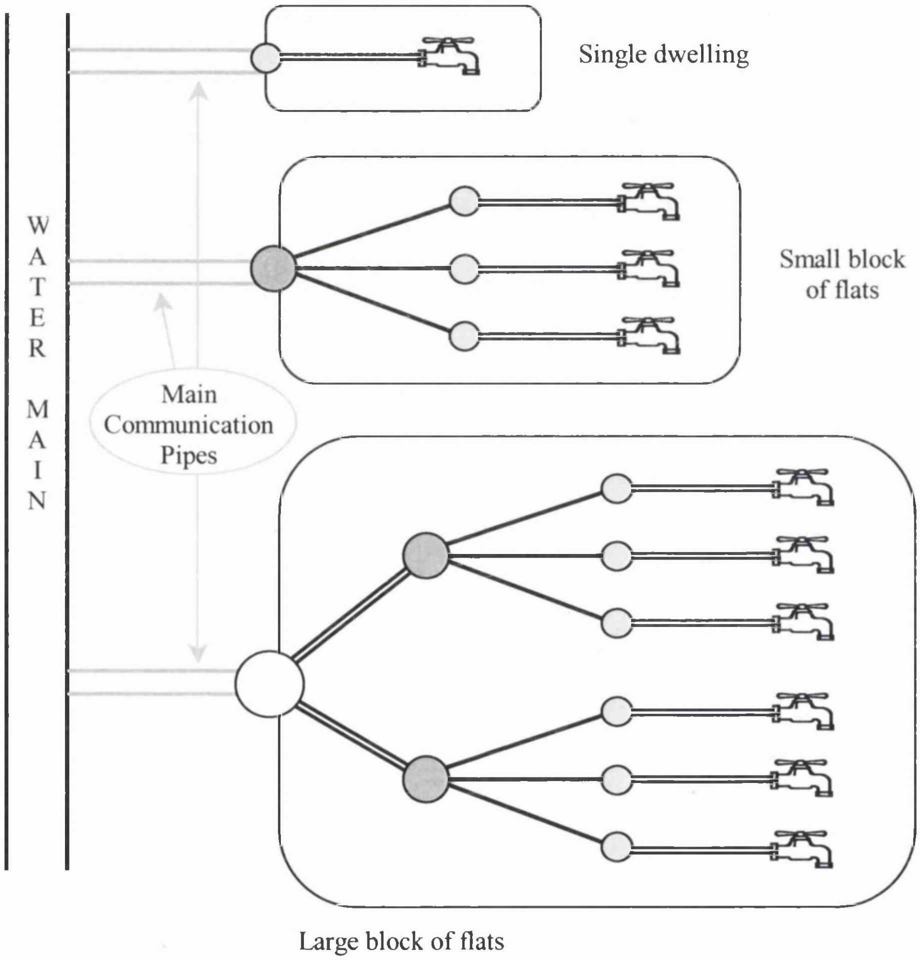

Figure 4.9. Connectivity in zone.

4.1.6.5 Pipework

The distribution of the lengths of the main communication pipes within the zone, obtained from survey data from the water company, is illustrated (Figure 4.10). It