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### **Paper:**

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# Multi-period Planning of a PVC Plant for the Optimization of Process Operation and Energy Consumption: An MINLP Approach

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**ABSTRACT:** This work addresses the integrated optimization of both the plant-wide material processing system and the utility system for a polyvinyl chloride (PVC) plant. In the plant-wide material processing system, vinyl chloride monomer (VCM) production process and VCM polymerization process **are** optimized to determine production allocation and switching operation of parallel equipment as well as raw material supply arrangement. In the utility system, power generation/supply plan is determined by combined heat and power (CHP) units and the state grid.

**The nonlinear electricity consuming characteristics of calcium carbide production process, CHP**

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3 process and electrolysis process are modeled based on the industrial data. A multi-period  
4 mixed-integer nonlinear programming (MINLP) model of a PVC plant by calcium carbide method  
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6 is proposed with the intent to enhance the profit and reduce the energy consumption. The proposed  
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8 MINLP model is successfully applied to two cases originated from a real-world industrial plant in  
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10 China and results provide valuable guidance for the company planning. The comparative results  
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12 verify the effectiveness and superiority of the proposed plant-wide integrated scheme.  
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19 **KEYWORDS:** Multiperiod Planning; PVC; Process Operation; Energy Consumption; MINLP.  
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## 23 1. INTRODUCTION

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25 Polyvinyl chloride (PVC) is a major commercial polymer and is widely used as a raw material in  
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27 various chemical and petrochemical products.<sup>1</sup> PVC production by calcium carbide method is  
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29 mainly adopted in China which accounts for 76.2% share, because of the abundance in coal and  
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31 shortage of gas and oil.<sup>2</sup> However, the calcium carbide method is known to be energy intensive,  
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33 resulting in high energy consumption, high cost and serious pollution problem. Process system  
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35 engineering methods, such as scheduling optimization and planning optimization, as effective  
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37 ways to promote profit have received increasing attention from both the academic and industrial  
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39 communities.  
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44 The scheduling problems of PVC polymerization process have been widely studied in the  
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46 literature. A multi-objective problem of scheduling and simulation technology aimed to the batch  
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48 or continuous production of a PVC factory was presented.<sup>3</sup> A software for on-line scheduling of  
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50 PVC suspension process including feed charging system, three parallel reactors as well as  
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52 discharge and cleaning operations was developed later.<sup>4</sup> An MILP scheduling model with batch  
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3 and continuous operations based on continuous time algorithm was studied in order to minimize  
4 the makespan for PVC polymerization.<sup>5</sup> Then a mixed integer linear programming (MILP) model  
5 for multistage polymer plants was introduced considering changeover cost, inventory cost and  
6 back-logging cost in PVC reaction, extrusion and packaging stages aiming at maximizing total  
7 profit.<sup>6</sup> Moreover, the problems of polymerizing production, storage, packaging, and  
8 transportation process for PVC process optimization were studied considering inventory cost and  
9 demand delay cost.<sup>1</sup> Integrated scheduling for PVC production considering calcium carbide  
10 production, brine electrolysis process and polymerization of VCM was studied and an MILP  
11 model was constructed.<sup>7-8</sup> The existing results of PVC production optimization mainly focused on  
12 PVC polymerization process to delivery process and few considered VCM production process.

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Many considerations for optimal operation or equipment transformation in calcium carbide production sector<sup>9-12</sup>, electrolysis sector<sup>13-16</sup> and CHP sector<sup>17-19</sup> have been addressed in order to save energy. The integrated optimization has been used in water supply system<sup>20</sup>, multi-product CSTRs<sup>21</sup> and biopharmaceutical manufacturing systems<sup>22</sup> that could provide further benefits than separate systems. However, to the best of our knowledge, the integrated planning optimization of both material processing system and utility system (mainly refers to CHP sector and state-grid procurement in this case) for a PVC plant is missing in the literature.

In this work, a multi-period mathematical model involving the process operation and energy consumption for planning optimization of a real-world PVC plant is presented. Nonlinear energy consumption characteristics for the most energy-intensive processes, i.e. calcium carbide furnaces, electrolytic cells and CHP units, are researched respectively. The nonlinear energy consumption models are then embedded into an MINLP planning model.

The rest of this paper is organized as follows. Firstly, a typical PVC production process is

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3 depicted in Section 2. Section 3 describes the optimization problem including energy and material  
4 consumption curves as well as equipment operation. The detailed plant-wide planning model is  
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6 elaborated in Section 4. Two cases from a real-world plant are presented to verify the feasibility of  
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8 the proposed MINLP model in Section 5, followed by conclusions in Section 6.  
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## 11 12 13 2. PROCESS DESCRIPTION

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15 The typical flowchart of the PVC production process by calcium carbide method is shown in  
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17 Figure 1. There are two systems, i.e. utility system and material processing system. In utility  
18 system, the electricity supply comes from CHP units and the state grid. In material processing  
19 system, PVC production is composed by two sequential parts: one is the VCM production and the  
20 second is VCM polymerization. Hydrogen ( $H_2$ ) and chlorine ( $Cl_2$ ) are made from brine  
21 electrolysis on the cathode and the anode respectively in electrolytic cells and burn together to  
22 produce hydrogen chloride (HCL) in a synthesis furnace after cooled and dried. Calcium carbide  
23 is made of coke and lime in calcium carbide furnaces and after well-cooled and crushed,  
24 combined with water to produce acetylene ( $C_2H_2$ ). HCL together with  $C_2H_2$  are mixed in  
25 proportion in the mixer. Then VCM is obtained by conversion of HCL and  $C_2H_2$ . After  
26 purification, compression and distillation, fresh VCM is stored in the storage tank to be used in  
27 the following polymerization process. Different grades of PVC are obtained from polymerization  
28 reactors under different temperatures, pressures and additives. Unreacted VCM is separated and  
29 recycled to the VCM tank. The final PVC is stored in the storage bin.  
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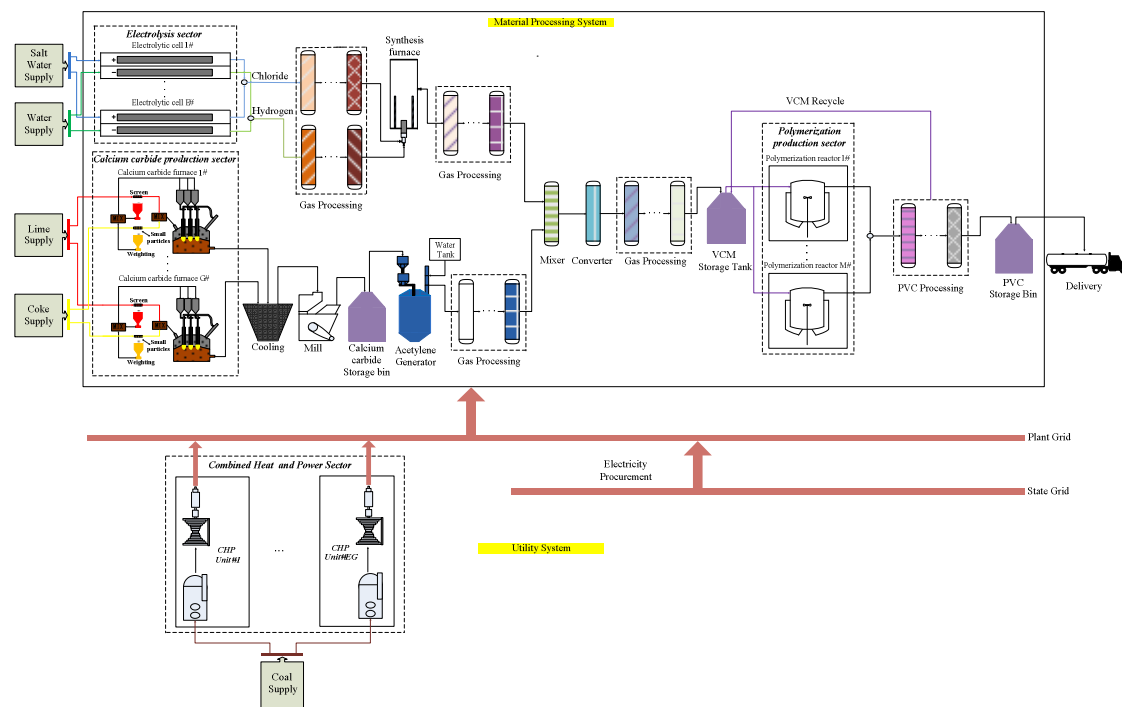
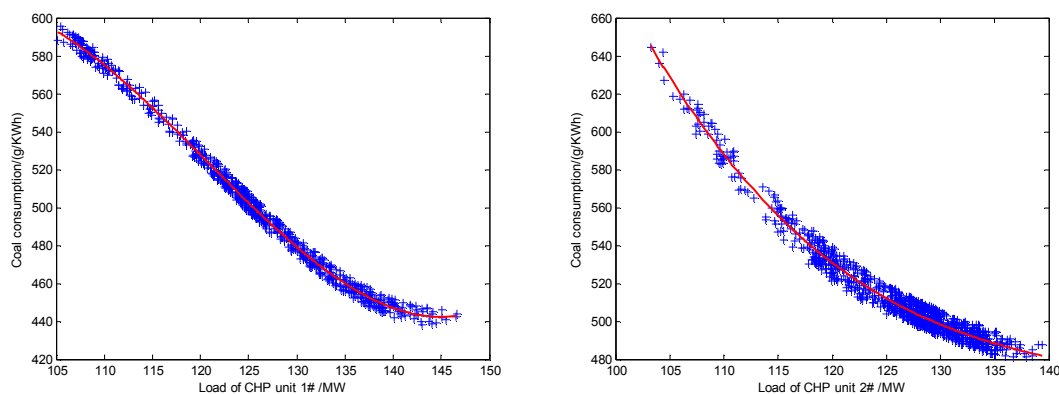


Figure 1. PVC production process.

### 3. PROBLEM STATEMENT

The whole process shown in Figure 1 is considered. The electricity consumed by material processing system is supplied by a plant grid, whose electricity comes from both CHP units and the state grid. Steady electricity procurement from the state grid is preferred for the sake of grid stability. Penalty is exerted for the procurement fluctuation case. Given the varying product demands, optimal balance between self-produced electricity from the CHP units and electricity procurement from the state grid should be determined to minimize the overall cost. The coal consumption in terms of the electricity load exhibits strong nonlinearity for CHP units, as shown in Figure 2. Moreover, there are distinct coal consumption characteristics for different CHP units. That is to say, a specific nonlinear correlation model can be driven from operational data for a particular CHP unit. A reasonable distribution of electricity load for these CHP units to reach minimum coal consumption is of vital importance for the energy and material saving. The

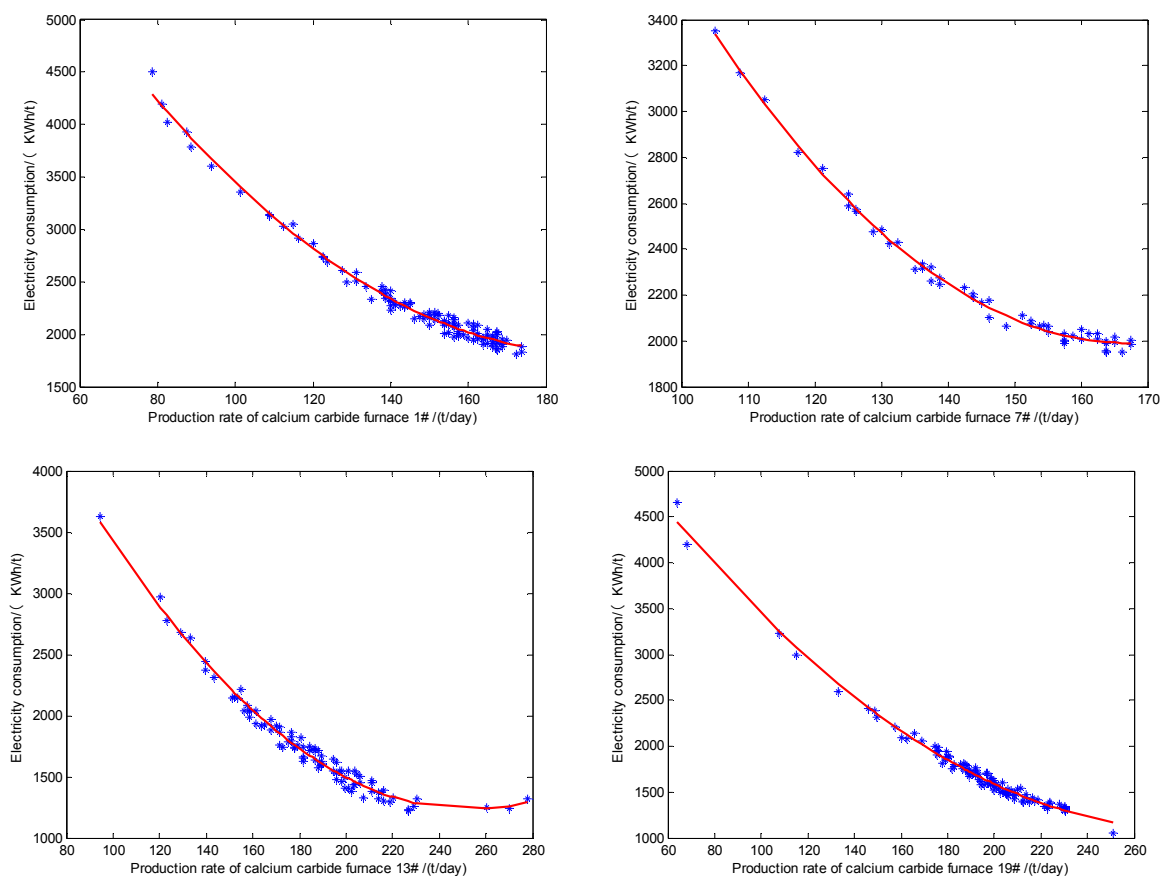
prediction curves in the red line shown in the paper are obtained by polynomial regression using the collected data from the plant. The regression model structure (i.e. the polynomial order) is determined based on its first principle model curve. Then, the data-driven model training method is used to obtain the model parameters optimally. The mathematical expressions and fitting accuracy, in term of relative sum of squared errors (RSSE), for these curves are given in Supporting Information S1-S3.



**Figure 2.** Coal consumption of CHP units with red line representing the prediction curve and blue cross points representing the collected data.

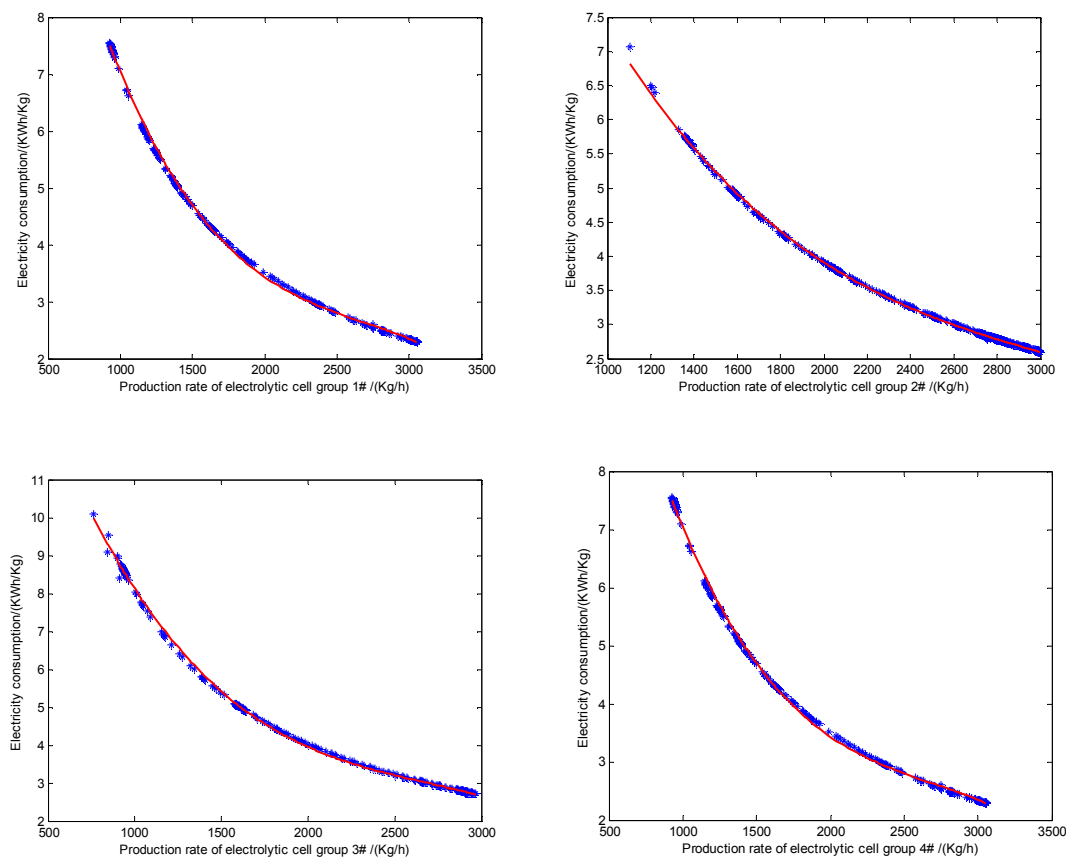
Calcium carbide process and chlorine production process account for nearly 75% energy consumption (i.e. mainly refers to the electricity consumption) of total plant.<sup>23</sup> Figure 3 shows the typical energy consumption in terms of calcium carbide production rate for each calcium carbide furnace. The detailed curves for electricity consumption of calcium carbide furnaces are shown in Supporting Information S2. As shown in Figure 3, it is clear that electricity consumption shows a nonlinear behavior. Multiple parallel calcium carbide furnaces with known processing capacities are utilized in a real-world plant, and moreover each furnace has its own particular electricity consumption characteristic. Therefore, under different production demands, there is large potential in electricity saving through optimally determining the working state and the

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4 production rate of calcium carbide furnaces. Similar with calcium carbide furnaces, electricity  
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6 consumption characteristics of electrolytic cells also present a high nonlinearity shown in Figure  
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9 4. The detailed functions and fitting accuracies of electrolytic cells are shown in Supporting  
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11 Information S3. All these nonlinear energy consumption models are addressed in this paper in  
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13 order of achieving the energy saving.  
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45 **Figure 3.** Electricity consumption of calcium carbide furnaces.  
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**Figure 4.** Electricity consumption of electrolytic cells.

When necessary, equipment should be shut down or restarted up to reduce energy consumption. But the frequent start-stop operation of **power-intensive equipment**, such as CHP units, calcium carbide furnaces and electrolytic cells, can cause the grid voltage sag. Voltage-sag is one of important factors having effect on electricity quality in supply system. Once the voltage sag is serious, **power-intensive equipment** in the system cannot work normally.<sup>24</sup> Therefore, frequent start-stop switches should be avoided and **operating state switches** should be penalized in the planning optimization.

The objective of this work is to propose a multi-period MINLP planning model considering various process operations and their energy consumption to optimally determine the plant-wide

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3 production arrangement plan, such as calcium carbide furnaces, electrolytic cells, polymerization  
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5 reactors and CHP units. Several assumptions are made in this study as follows:  
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8 (1) Only electricity consumption is considered in this study, partly because electricity is the  
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10 major energy form compared to other energy, such as steam water and so on, and partly because  
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12 there is much more potential to optimize the electricity.  
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15 (2) The impact of coal composition variation is ignored.  
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18 (3) The calcium carbide produced from different furnaces has the same quality, i.e. the same  
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20 gas yield level. Because the quality variation caused by the operating conditions is small enough  
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22 to be ignored for planning issue.  
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25 Those assumptions are approximately held in reality. Based on these assumptions, the  
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27 mathematical model for this planning issue is detailed in the next section.  
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30 Given:

31 (1) A planning horizon and planning period;

32 (2) A set of demands for each grade of PVC along the planning horizon;

33 (3) A set of process units such as calcium carbide furnaces, electrolytic cells, polymerization  
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35 reactors and CHP units and their working load range;  
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39 (4) A set of storage bins and their minimum and maximum stock;

40 (5) A set of components and their initial inventories;

41 (6) Market price of raw materials, inventory and electricity from the state grid;

42 (7) The penalty of switching operations and stockout.  
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46 To determine:

47 (1) The type of PVC and production amount in each polymerization reactor in each time  
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49 period.  
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(2) The production rate and operating state of calcium carbide furnaces, electrolytic cells, polymerization reactors and CHP units.

(3) The detailed supply of materials.

So as to:

Minimize the total cost, including the costs of raw materials, inventory, electricity consumption, the penalty of stockout and start-stop(start-up and shutdown) switching.

#### 4. MATHEMATICAL MODEL

The plant-wide planning model defined as a multi-period MINLP has been modeled considering both material processing system and electricity generation/supply system.

##### 4.1 Model of Delivery and PVC Storage

The inventory balance and inventory capacity constraints for different grades of PVC are expressed in equations 1 and 2 respectively. Equation 1 shows that final PVC inventory  $MI_{i,w}$  is given as the balance on the previous inventory level  $MI_{i,w-1}$  plus polymerization production amount  $PT_{i,u,w}$  minus delivery amount  $S_{i,w}$ . Equation 2 forces the current inventory level of  $i$  product to be bounded between minimum inventory capacity  $MI_i^{min}$  and maximum inventory capacity  $MI_i^{max}$ .

$$MI_{i,w} = MI_{i,w-1} + \sum_{u \in M} PT_{i,u,w} - S_{i,w} \quad \forall i \in MP, w \in W \quad (1)$$

$$MI_i^{min} \leq MI_{i,w} \leq MI_i^{max} \quad \forall i \in MP, w \in W \quad (2)$$

PVC's delivery should be no more than the demand, as shown in equation 3, so stockout state of PVC is considered. Penalty factor is introduced in the objective function for stockout state.

$$S_{i,w} \leq D_{i,w} \quad \forall i \in MP, w \in W \quad (3)$$

where  $D_{i,w}$  represents the market demand of PVC  $i$  during  $w$  week.

## 4.2 Polymerization Process Model

According to market demands and inventory requirements,  $PT_{i,u,w}$  which denotes production for grade  $i$  in polymerization reactor  $u$  during  $w$  week, shown in equation 4, should be determined firstly. Polymerization process is operated in a batch-wise manner with  $cy$  hours discharge period. Each polymerization reactor has its own fixed feeding quantity  $FS_u$ . Besides, taking one week as a planning period, the number of feeding batches  $N_{i,u,w}$  is limited by equation 5.

$$PT_{i,u,w} = N_{i,u,w} * FS_u * \alpha_{i,u} \quad \forall i \in MP, u \in M, w \in W \quad (4)$$

$$0 \leq \sum_{i \in MP} N_{i,u,w} \leq \frac{168}{cy} \quad \forall u \in M, w \in W \quad (5)$$

where  $\alpha_{i,u}$  denotes conversion rate of VCM to the PVC product  $i$  in the polymerization reactor  $u$ .

## 4.3 VCM Process Model

According to the production of PVC, the corresponding consumption of VCM is expressed in equation 6. From the process flowchart, VCM is synthesized by HCL and  $C_2H_2$ . According to the strict chemical principle balance equation, the relationship between VCM, HCL and  $C_2H_2$  is formulated in equations 7-8. The inventory constraints of VCM are expressed in equations 9-10.

$$CM_{vcm,w} = \sum_{u \in M} \sum_{i \in MP} N_{i,u,w} * FS_u \quad \forall w \in W \quad (6)$$

$$PT_{vcm,w} = CM_{Hcl,w} + CM_{C_2H_2,w} \quad \forall w \in W \quad (7)$$

$$\frac{CM_{Hcl,w}}{36.5} = \frac{CM_{C_2H_2,w}}{26} \quad \forall w \in W \quad (8)$$

$$MI_{vcm,w} = MI_{vcm,w-1} + PT_{vcm,w} - CM_{vcm,w} \quad \forall w \in W \quad (9)$$

$$MI_{vcm}^{min} \leq MI_{vcm,w} \leq MI_{vcm}^{max} \quad \forall w \in W \quad (10)$$

#### 4.4 C<sub>2</sub>H<sub>2</sub> and HCL Process Model

HCL is synthesized by Cl<sub>2</sub> and H<sub>2</sub>, while C<sub>2</sub>H<sub>2</sub> is obtained from CaC<sub>2</sub>. The planning optimization is medium or long term from weeks, months to years. For that time scale, the reaction process can be considered as complete and ideal. Then the output of HCL is proportional to the consumption of Cl<sub>2</sub> while C<sub>2</sub>H<sub>2</sub> is proportional to the consumption of CaC<sub>2</sub>, as shown in equations 11-12. The inventory capacity of gas holder for C<sub>2</sub>H<sub>2</sub> in reality is very limited and can be ignored, so we can consider that the output of C<sub>2</sub>H<sub>2</sub> is equal to the consumption of C<sub>2</sub>H<sub>2</sub> shown in equation 13.

$$CM_{HCl,w} = \gamma * CM_{Cl_2,w} \quad \forall w \in W \quad (11)$$

$$PT_{C_2H_2,w} = \beta * CM_{CaC_2,w} \quad \forall w \in W \quad (12)$$

$$PT_{C_2H_2,w} = CM_{C_2H_2,w} \quad \forall w \in W \quad (13)$$

where  $\gamma$  denotes the transfer coefficient for output of HCL and consumption of Cl<sub>2</sub>,  $\beta$  denotes the transfer coefficient for output of C<sub>2</sub>H<sub>2</sub> and consumption of CaC<sub>2</sub>.

#### 4.5 Chlorine Process Model

Chlorine production is the primary step of PVC production process shown in equations 14-16. Multiple parallel electrolytic cells with specific electricity consumption characteristics are considered. The output of Cl<sub>2</sub> is related to electrolytic cells' working state  $Z_{u,w}$ , production rate  $P_{Cl_2,u,w}$  and production time  $T_{Cl_2}$ . In a real chemical plant, production rate of Cl<sub>2</sub> should be restricted in a reasonable range shown in equation 15. Moreover, chlorine production process is continuous with limited inventory, so the output of Cl<sub>2</sub> can be equal to the consumption of Cl<sub>2</sub> in equation 16.

$$PT_{cl2,u,w} = Z_{u,w} * P_{cl2,u,w} * T_{cl2} \quad \forall u \in E, w \in W \quad (14)$$

$$P_{cl2,u,w}^{min} * Z_{u,w} \leq P_{cl2,u,w} \leq P_{cl2,u,w}^{max} * Z_{u,w} \quad \forall u \in E, w \in W \quad (15)$$

$$\sum_{u \in E} PT_{cl2,u,w} = CM_{cl2,w} \quad \forall w \in W \quad (16)$$

It's clear that equation 14 is a bilinear term. We linearize it based on the method proposed by You and Grossmann<sup>25</sup>. By introducing two auxiliary variables  $ZP_{cl2,u,w}$  and  $AX_{cl2,u,w}$ , the equation 14 can be replaced as following equations (14-1) to (14-5).  $P_{cl2,u,w}^{max}$  is defined as maximum production rate of  $Cl_2$  for equipment  $u$  in  $w$  week. Equations 17 and 24 are handled using the same methods.

$$PT_{cl2,u,w} = ZP_{cl2,u,w} * T_{cl2} \quad \forall u \in E, w \in W \quad (14-1)$$

$$ZP_{cl2,u,w} + AX_{cl2,u,w} = P_{cl2,u,w} \quad \forall u \in E, w \in W \quad (14-2)$$

$$ZP_{cl2,u,w} \leq Z_{u,w} * P_{cl2,u,w}^{max} \quad \forall u \in E, w \in W \quad (14-3)$$

$$AX_{cl2,u,w} \leq (1 - Z_{u,w}) * P_{cl2,u,w}^{max} \quad \forall u \in E, w \in W \quad (14-4)$$

$$ZP_{cl2,u,w} \geq 0, AX_{cl2,u,w} \geq 0 \quad \forall u \in E, w \in W \quad (14-5)$$

#### 4.6 Calcium Carbide Production Process

Calcium carbide production can be seen as a continuous process. The production is expressed in equation 17 which is related to calcium carbide furnaces' working state  $Z_{u,w}$ , production rate  $P_{cac2,u,w}$  and production time  $T_{cac2}$ . The limit for production rate of calcium carbide furnaces is expressed in equation 18. Calcium carbide is stored in storage bin and inventory limit is expressed in equations 19-20.

$$PT_{cac2,u,w} = Z_{u,w} * P_{cac2,u,w} * T_{cac2} \quad \forall u \in G, w \in W \quad (17)$$

$$P_{cac2,u,w}^{min} * Z_{u,w} \leq P_{cac2,u,w} \leq P_{cac2,u,w}^{max} * Z_{u,w} \quad \forall u \in G, w \in W \quad (18)$$

$$MI_{cac2,w} = MI_{cac2,w-1} + \sum_{u \in EG} PT_{cac2,u,w} - CM_{cac2,w} \quad \forall w \in W \quad (19)$$

$$MI_{cac2}^{min} \leq MI_{cac2,w} \leq MI_{cac2}^{max} \quad \forall w \in W \quad (20)$$

#### 4.7 Power Consumption and Generation

In this paper, the electricity consumption of calcium carbide furnaces and electrolytic cells are the main energy consumption form of the total plant. The nonlinear relationship between electricity consumption and production rate of  $Cl_2$  or  $CaC_2$  is given respectively in Section 3.  $f_u(P_{cac2,u,w})$  and  $f_u(P_{cl2,u,w})$  are models of Figure 3 and 4 respectively. Therefore, the total electricity consumption  $ele_w$  is calculated in equation 21. Besides, the plant grid supplies electricity for the plant-wide production process, as shown in equation 22. To satisfy the demand of the electricity consumption, electricity supply should be restricted in equation 23. The electricity supply of CHP units is constrained by equations 24-25. The production load of CHP units is determined by working state  $Z_{u,w}$ , power  $PW_{u,w}$  which is restricted by minimum and maximum power, and running time  $T_{CHP}$ .

$$ele_w = \sum_{u \in E} f_u(P_{cl2,u,w}) * PT_{cl2,u,w} + \sum_{u \in EG} f_u(P_{cac2,u,w}) * PT_{cac2,u,w} \quad \forall w \in W \quad (21)$$

$$elesp_w = \sum_{u \in EG} PE_{u,w} + SG_w \quad \forall w \in W \quad (22)$$

$$elesp_w \geq ele_w \quad \forall w \in W \quad (23)$$

$$PE_{u,w} = Z_{u,w} * PW_{u,w} * T_{CHP} \quad \forall u \in EG, w \in W \quad (24)$$

$$PW_{u,w}^{min} * Z_{u,w} \leq PW_{u,w} \leq PW_{u,w}^{max} * Z_{u,w} \quad \forall u \in EG, w \in W \quad (25)$$

#### 4.8 Raw Material Constraints

The inventory balance and inventory capacity constraint for raw materials are shown in

equations 26-27 respectively. Equations 28-31 denote the consumption of each raw material. The coal consumption is nonlinear with the load of CHP units as Section 3 presented.  $f_u(Pw_{u,w})$  is the model in Figure 2.

$$MI_{r,w} = MI_{r,w-1} + SP_{r,w} - Cm_{r,w} \quad \forall r \in MR, w \in W \quad (26)$$

$$MI_r^{min} \leq MI_{r,w} \leq MI_r^{max} \quad \forall r \in MR, w \in W \quad (27)$$

$$CM_{coke,w} = \delta * \sum_{u \in G} PT_{cac2,u,w} \quad \forall w \in W \quad (28)$$

$$CM_{cao,w} = \varepsilon * \sum_{u \in G} PT_{cac2,u,w} \quad \forall w \in W \quad (29)$$

$$CM_{Nacl,w} = \epsilon * \sum_{u \in E} PT_{cl2,u,w} \quad \forall w \in W \quad (30)$$

$$CM_{coal,w} = \sum_{u \in EG} f_u(Pw_{u,w}) * PE_{u,w} \quad \forall w \in W \quad (31)$$

where  $\delta$  denotes the transfer coefficient for output of  $CaC_2$  and consumption of coke;  $\varepsilon$  denotes the transfer coefficient for output of  $CaC_2$  and consumption of  $CaO$ ;  $\epsilon$  denotes the transfer coefficient for output of  $Cl_2$  and consumption of salt.

#### 4.9 Start-Stop Operation of Calcium Carbide Furnaces, Electrolytic Cells and CHP Units

Frequent start-stop operations affect the manufacturing process and cause excessive but unnecessary energy loss, which should be minimized. The binary variable  $ZF_{u,w}=1$  denotes the occurrence of start-stop operation in u equipment during w week and w+1 week. The binary variable  $Z_{u,w}=1$  denotes working state of u equipment in w week;  $Z_{u,w}=0$  means idle state of u equipment in w week. Clearly, if there is no working state switch, i.e.  $Z_{u,w} = Z_{u,w+1}$ , the state switching variable  $ZF_{u,w}$  will be zero because it is penalized in objective function. However, if there is working state switch, which means that  $Z_{u,w} \neq Z_{u,w+1}$ , i.e.  $Z_{u,w} = 1, Z_{u,w+1} = 0$  or  $Z_{u,w} = 0, Z_{u,w+1} = 1$ ,  $ZF_{u,w}$  will be one to follow the constraints 32-33.

$$ZF_{u,w} + Z_{u,w+1} \geq Z_{u,w} \quad \forall u \in FA, w \in W \quad (32)$$



$$ZF_{u,w} + Z_{u,w} \geq Z_{u,w+1} \quad \forall u \in FA, w \in W \quad (33)$$

#### 4.10 Objective Function

The objective described in equation 34 aims at minimizing the overall cost, which includes the costs of raw materials (i.e. coke, coal, salt and lime), stockout penalty, inventory (i.e. PVC inventory, VCM inventory, calcium carbide inventory and raw material inventory), the start-stop switching penalty and electricity consumption.

$$cost = \left\{ \begin{array}{l} \sum_{i \in MR} \sum_{w \in W} CRM_r * SP_{r,w} + \sum_{i \in MP} \sum_{w \in W} Py_i * (D_{i,w} - S_{i,w}) + \\ \sum_{w \in W} \sum_{i \in MP} CI_i * MI_{i,w} + \sum_{w \in W} \sum_{r \in MR} CI_r * MI_{r,w} + \sum_{w \in W} CI_{vcm} * MI_{vcm,w} \\ + \sum_{w \in W} CI_{cac2} * MI_{cac2,w} + \sum_{u \in FA} \sum_{w \in W} CF_u * ZF_{u,w} + CE * \sum_{w \in W} SG_w \end{array} \right. \quad (34)$$

where  $CRM_r$  denotes the price of raw material  $r$ ;  $Py_i$  is stockout punishment for product  $i$ ;  $CI_i$ ,  $CI_r$ ,  $CI_{vcm}$  and  $CI_{cac2}$  is inventory cost for PVC product  $i$ , raw material  $r$ , VCM and  $CaC_2$  respectively;  $CF_u$  denotes start-stop operation cost for equipment  $u$ ;  $CE$  is the price of procurement electricity from the state grid.

### 5. CASE STUDY

To verify the applicability of proposed model, two planning optimization cases originated from a real-world PVC plant in China are provided here, which has 20 polymerization reactors, 20 calcium carbide furnaces and 4 groups' electrolytic cells with 6 pieces in each group. The weekly demands of five different PVC products are shown in Table 1 for a time horizon of 12 weeks. The parameters used in the model are shown in Supporting Information S4.

The entire model is computed by GAMS win 32 24.0.2 and solved by the solver of ALPHAECP in an Intel Xeon CPU, 3.5GHz machine with 64GB of RAM.

Table 1. Weekly demands (ton)

	Products	Weekly demands						
		1	2	3	4	5	6	
Case 1	A	2100	1500	5500	2700	1500	4500	
	B	3500	2800	3000	1500	4900	1500	
	C	3200	2700	1500	6200	3700	1500	
	D	2700	2000	6000	4500	1500	1500	
	E	2700	3400	1500	2600	5000	6200	
		Products	Weekly demands					
			7	8	9	10	11	12
		A	2500	2500	4000	3000	2700	1500
		B	1500	3800	1500	2400	2500	3300
		C	3900	2700	1500	4000	2200	3500
	D	5800	1500	6500	1500	4400	5950	
	E	1500	3700	2000	2900	3400	1500	
Case 2		Products	Weekly demands					
			1	2	3	4	5	6
		A	8000	2000	8000	2500	1000	2000
		B	2000	6000	1000	2500	3000	0
		C	1600	0	1500	6500	5000	0
		D	0	5000	0	4000	1000	0
		E	2600	0	7000	2000	6000	8000
		Products	Weekly demands					
			7	8	9	10	11	12
		A	4000	1000	1000	1000	1400	0
	B	0	3000	1000	6500	1200	3600	
	C	3000	1000	4200	2000	2600	2000	
	D	500	3000	0	0	2000	2000	
	E	5000	1000	6000	1800	9800	8000	

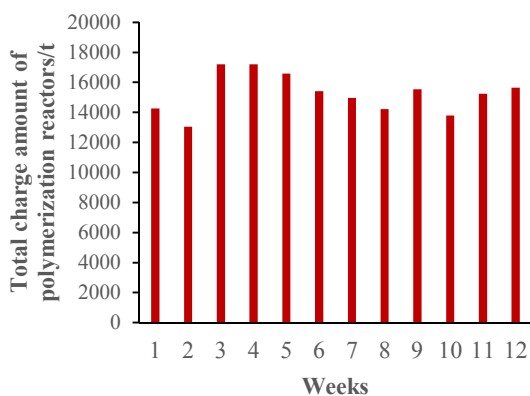
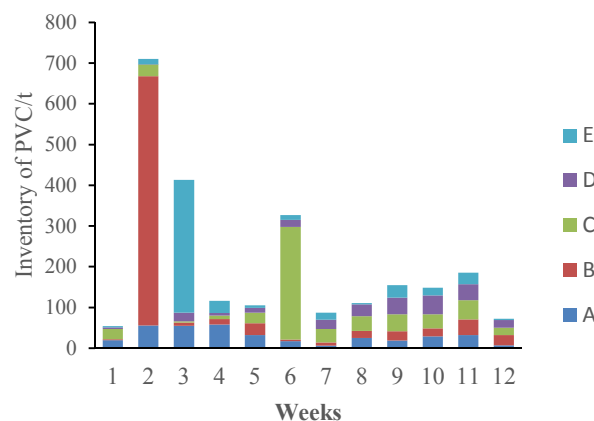
The model statistics are shown in Table 2. The optimality tolerance is set to 1% and the computational time limit is set to 4 hours for these two models to make a fair comparison. From Table 2, it is clear that the separate model method can obtain the result with the lower optimality gap, because several small-scale and thus easy-to-solve sub-models are solved for this method comparing with the integrated model method. How to reduce the optimality gap and improve the solution quality of the proposed integrated model is under our further research.

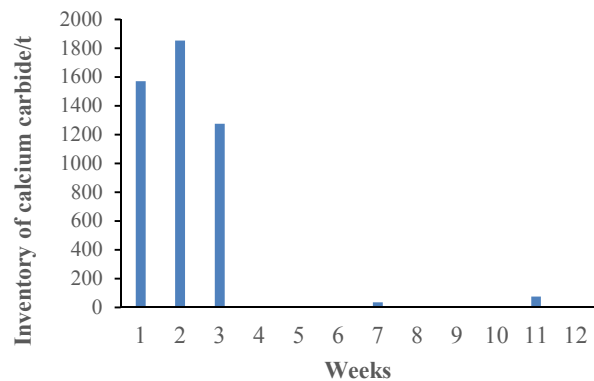
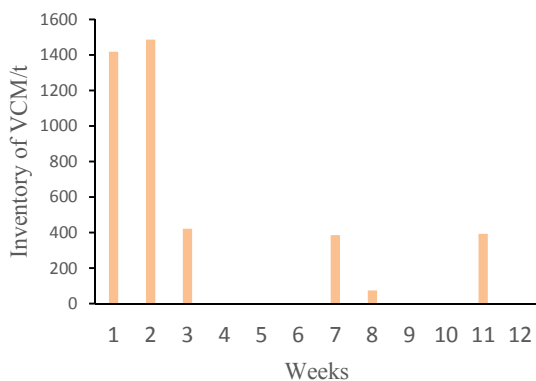
**Table 2. Model statistics**

Case	Model	Equations	Discrete Variable Number	Continuous Variable Number	CPU Time(s)	Optimality GAP(%)
		Case 1	Integrated model	6,694	2,304	4,254
Case 1	Separate model	6,753	2,304	4,313	14,400	1
Case 2	Integrated model	6,695	2,304	4,255	14,400	10
Case 2	Separate model	6,830	2,304	4,526	14,400	1

### 5.1 Results Explanation of Case 1

Case 1 is used to explain the detailed results of proposed model. The total cost is 166,392,500 CNY. The total charge amount of polymerization reactors is shown in Figure 5 and the inventory of PVC is depicted in Figure 6. From the analysis of Figure 5 and 6, production of PVC meets the given demands and no stockout occurs. All polymerization reactors produce 17,203.2 t per week at full capacity. The total demands in the 3<sup>rd</sup> and 4<sup>th</sup> weeks exceed the maximum production of the plant. In order to satisfy the demands in the 3<sup>rd</sup> and 4<sup>th</sup> weeks, the inventory of PVC in the 2<sup>nd</sup> and 3<sup>rd</sup> weeks is large. The inventory of VCM and calcium carbide are shown in Figure 7 and 8 respectively. The **detailed** production of polymerization reactors is shown in Figure 9.

**Figure 5.** Total charge amount of polymerization reactors**Figure 6.** The inventory of PVC.

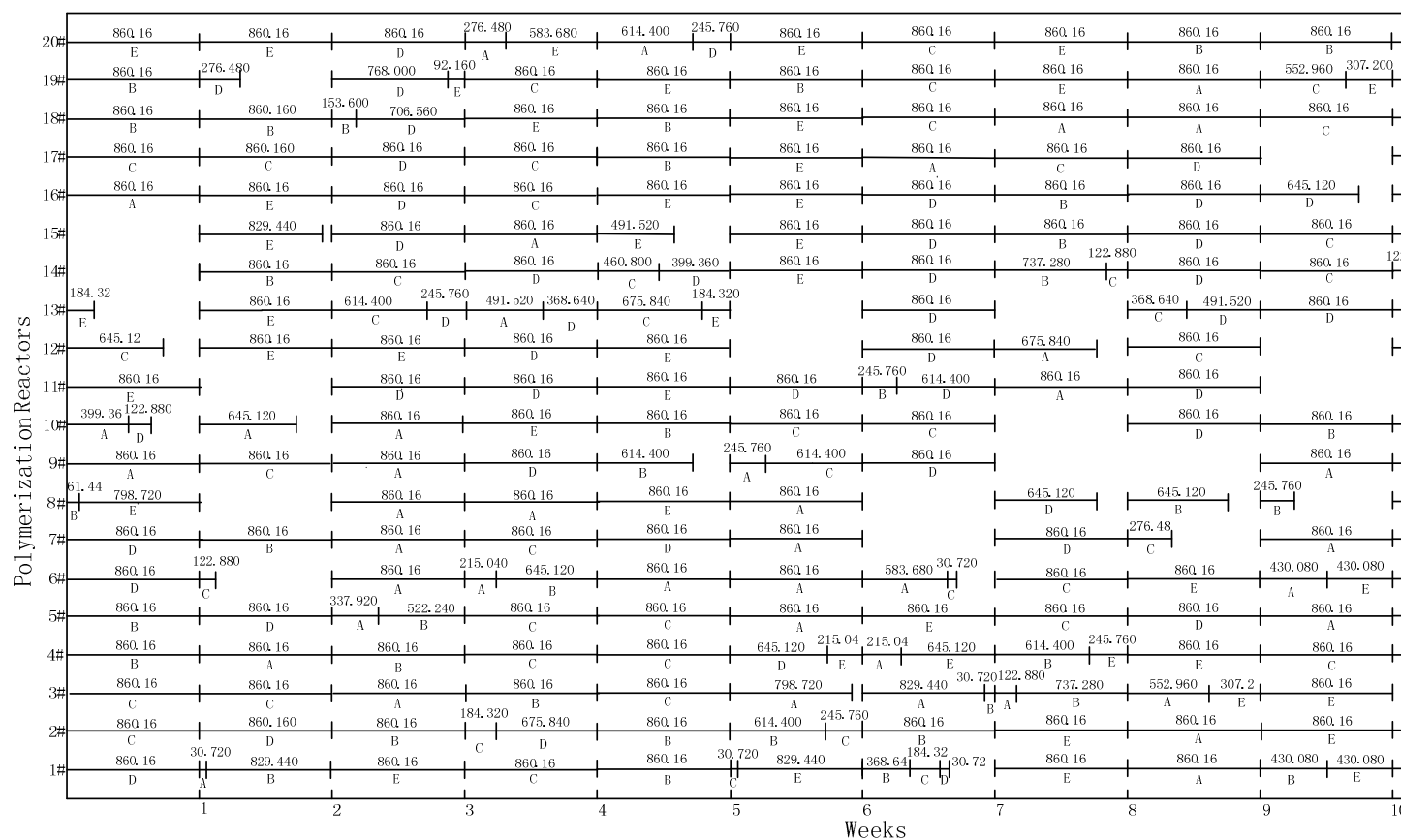


**Figure 7.** The inventory of VCM.

**Figure 8.** The inventory of calcium carbide.

The working states of calcium carbide furnaces during the planning time horizon are shown in Table 3. Calcium carbide furnaces 2# and 7# are idle during the planning horizon. However, calcium carbide furnaces 12#, 16# and 19# keep working in 12 weeks. There are start-stop operations for the rest of calcium carbide furnaces. As we can see, the start-stop operations of calcium carbide furnaces are frequent because of the tradeoff among the electricity consumption, the production of calcium carbide and switching operation cost. Typical production rate curves of calcium carbide furnaces are shown in Figure 10 and detailed curves are given in Supporting Information S5. Figure 10(a) shows that the calcium carbide furnace is not working while the calcium carbide furnace in Figure 10(b) works at full capacity during the planning horizon. The calcium carbide furnace in Figure 10(c) also works during the horizon but the production rate changes. There exist start-stop operations shown in Figure 10(d).

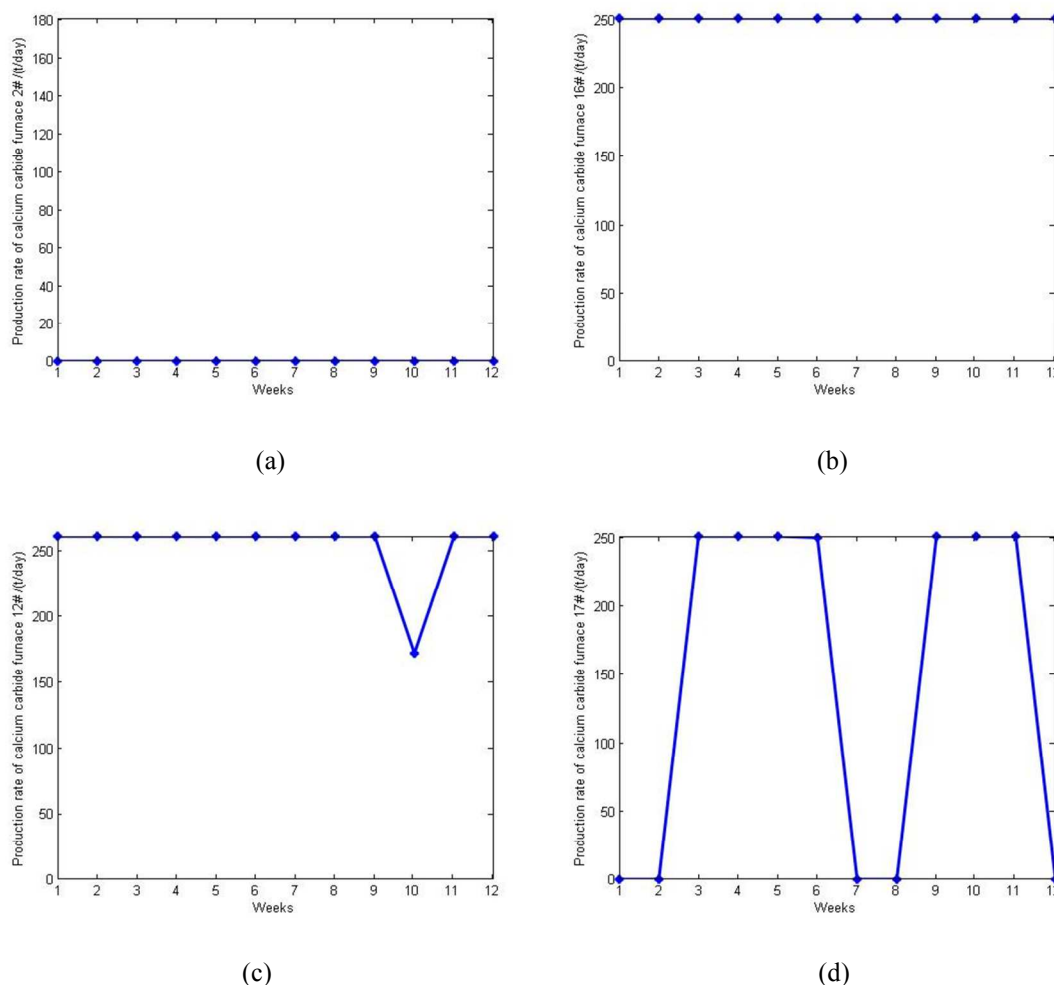
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**Figure 9.** Planning production of polymerization reactors.

**Table 3. Working state of calcium carbide furnaces: grey box representing the used furnace and blank box representing the idle furnace**

Calcium carbide furnace	1 <sup>st</sup> week	2 <sup>nd</sup> week	3 <sup>rd</sup> week	4 <sup>th</sup> week	5 <sup>th</sup> week	6 <sup>th</sup> week	7 <sup>th</sup> week	8 <sup>th</sup> week	9 <sup>th</sup> week	10 <sup>th</sup> week	11 <sup>th</sup> week	12 <sup>th</sup> week
1#			■		■						■	
2#												
3#		■	■	■	■	■	■	■			■	■
4#	■		■	■			■		■	■		■
5#								■				
6#			■		■	■	■		■			■
7#												
8#	■							■				
9#	■		■									
10#	■	■		■	■	■	■	■			■	
11#	■			■	■							
12#	■	■	■	■	■	■	■	■	■	■	■	■
13#			■							■		
14#	■	■		■	■	■	■	■	■	■	■	■
15#											■	■
16#	■	■	■	■	■	■	■	■	■	■	■	■
17#			■	■	■	■			■	■	■	
18#	■	■	■	■		■	■	■	■	■	■	■
19#	■	■	■	■	■	■	■	■	■	■	■	■
20#	■	■	■	■	■	■	■	■	■	■		■



**Figure 10.** Production rate curves of different calcium carbide furnaces.

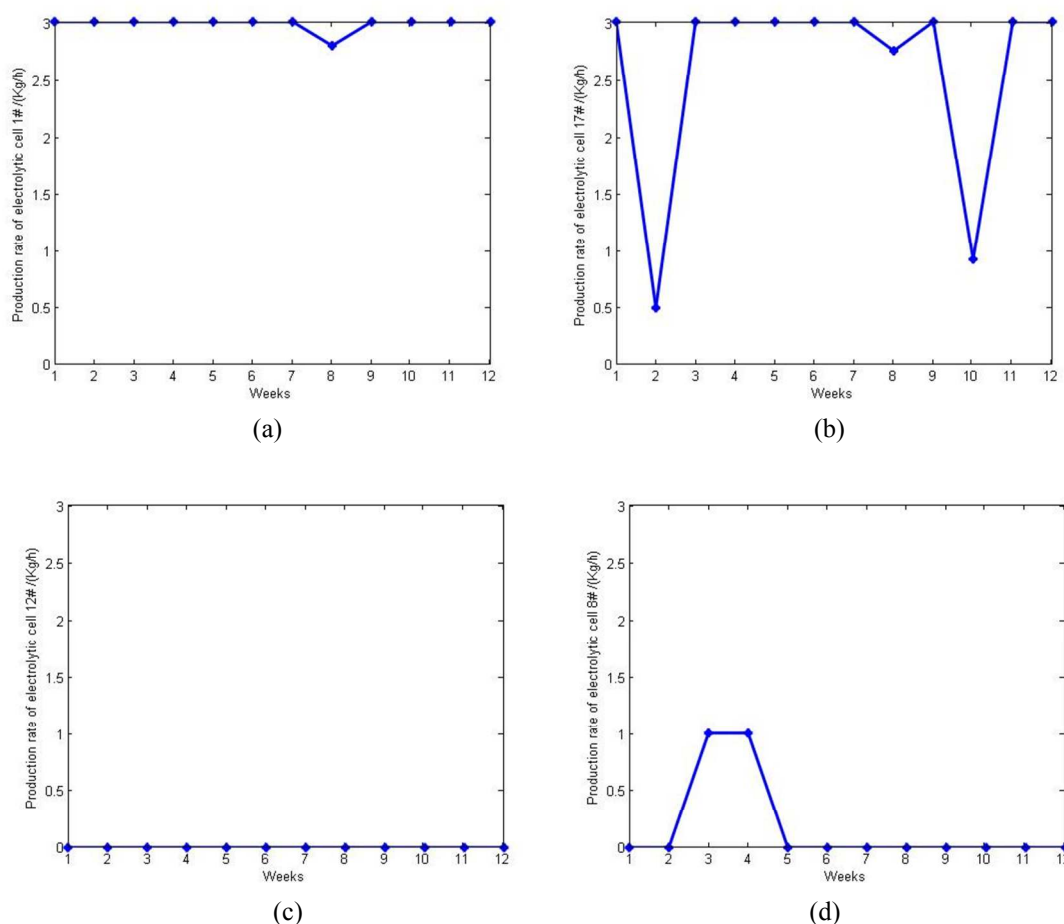
The working states of electrolytic cells during the planning time horizon are shown in Table 4. As we can see, electrolytic cells 1#-6# and 13#-24# are working while 11# and 12# are idle during the horizon. Electrolytic cell 7# works in the 1<sup>st</sup> week and then shuts down in the 2<sup>nd</sup> week. Electrolytic cells 7#-9# start up in the 3<sup>rd</sup> week and shut down in the 6<sup>th</sup>, 4<sup>th</sup> and 5<sup>th</sup> weeks respectively. Electrolytic cell 10# starts up in the 9<sup>th</sup> week and works until the end of the horizon. The typical production rate curves of electrolytic cells are shown in Figure 11 and the detailed curves are shown in Supporting Information S6. The lowest production rate is 1t/h for electrolytic cells 6#-12# and the rest is 0.5t/h. The highest production rate is 3t/h for all

1  
2  
3 electrolytic cells. Figure 11(a) and 11(b) show that the electrolytic cells work during the horizon  
4 and the production rate can change. Figure 11(c) shows the idle situation of electrolytic cells and  
5  
6  
7  
8 Figure 11(d) performs start-stop switching operations.

9  
10 **Table 4. Working state of electrolytic cells: grey box representing the used cell and blank box**  
11 **representing the idle cell**

Electrolytic cell	1st week	2nd week	3rd week	4th week	5th week	6th week	7th week	8th week	9th week	10th week	11th week	12th week
1#	■	■	■	■	■	■	■	■	■	■	■	■
2#	■	■	■	■	■	■	■	■	■	■	■	■
3#	■	■	■	■	■	■	■	■	■	■	■	■
4#	■	■	■	■	■	■	■	■	■	■	■	■
5#	■	■	■	■	■	■	■	■	■	■	■	■
6#	■	■	■	■	■	■	■	■	■	■	■	■
7#	■		■	■	■	■	■					
8#			■	■								
9#			■	■	■	■						
10#									■	■	■	■
11#												
12#												
13#	■	■	■	■	■	■	■	■	■	■	■	■
14#	■	■	■	■	■	■	■	■	■	■	■	■
15#	■	■	■	■	■	■	■	■	■	■	■	■
16#	■	■	■	■	■	■	■	■	■	■	■	■
17#	■	■	■	■	■	■	■	■	■	■	■	■
18#	■	■	■	■	■	■	■	■	■	■	■	■
19#	■	■	■	■	■	■	■	■	■	■	■	■
20#	■	■	■	■	■	■	■	■	■	■	■	■
21#	■	■	■	■	■	■	■	■	■	■	■	■
22#	■	■	■	■	■	■	■	■	■	■	■	■
23#	■	■	■	■	■	■	■	■	■	■	■	■
24#	■	■	■	■	■	■	■	■	■	■	■	■





**Figure 11.** Production rate curves of different electrolytic cells.

The power of CHP units is shown in Figure 12. Electricity consumption and supply are shown in Table 5. The maximum power of CHP unit 1# and CHP unit 2# are 145MW and 140MW respectively. The minimum power of CHP 1# and CHP 2# are 105MW and 100MW respectively. Two CHP units work simultaneously during the horizon, so there is no start-stop switching operation. In the 3<sup>rd</sup> and 4<sup>th</sup> weeks, two CHP units work at full capacity and electricity procurement is also needed. In the rest of weeks, the electricity generated from CHP units meets electricity consumption from the plant-wide material processing process and there is no need to purchase electricity from the state grid.

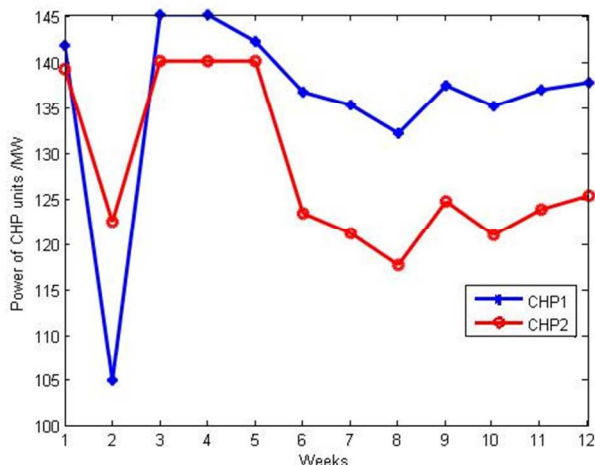


Figure 12. CHP unit power.

Table 5. Electricity consumption and supply (KW • h)

Items	1 <sup>st</sup> week	2 <sup>nd</sup> week	3 <sup>rd</sup> week	4 <sup>th</sup> week	5 <sup>th</sup> week	6 <sup>th</sup> week
Electricity Consumption	47,176,637	38,207,456	52,224,315	49,296,864	47,394,944	43,675,751
Electricity Supply from CHP units	47,176,637	38,207,456	47,880,000	47,880,000	47,394,944	43,675,751
Electricity Procurement	0	0	4,344,315	1,416,864	0	0
Items	7 <sup>th</sup> week	8 <sup>th</sup> week	9 <sup>th</sup> week	10 <sup>th</sup> week	11 <sup>th</sup> week	12 <sup>th</sup> week
Electricity Consumption	43,062,759	41,954,290	44,015,571	43,006,901	43,787,455	44,175,583
Electricity Supply from CHP units	43,062,759	41,954,290	44,015,571	43,006,901	43,787,455	44,175,583
Electricity Procurement	0	0	0	0	0	0

## 5.2 Comparative results

To verify the effectiveness of integrated model we proposed above, the model is compared to the separate model, i.e. polymerization reactor sector, electrolytic cell sector, calcium carbide sector and utility system respectively. The total cost includes energy cost, inventory cost,

1  
2  
3 material cost, **stockout cost** and switching cost. Energy cost includes electricity procurement cost  
4  
5 and coal consumption cost.  
6

7  
8 Table 6 and 7 show the comparisons between the integrated model and the **separate** models.  
9  
10 From the data listed in the Table 6, it's clear that the integrated model is superior to the separate  
11  
12 model in total cost and energy cost. The total cost of integrated model is 2.6% less than the  
13  
14 separate model. The energy cost of integrated model decreases 5.1% compared to the separate  
15  
16 model. **The main reason for energy saving is the truth that the integrated model has the potential**  
17  
18 **to optimize it in a global horizon. The integrated model globally pursues the working state and**  
19  
20 **production rate of units as optimal as possible to reduce their energy cost. The result shows that**  
21  
22 **the switching cost of integrated model is more than the separate model. Due to the varying PVC**  
23  
24 **demands in each weeks, the integrated model will compromise between the switching cost,**  
25  
26 **inventory cost and each units' energy cost and choose the optimal production rates in most**  
27  
28 **appropriate units that may lead to large switching cost.**  
29  
30  
31  
32  
33

34 From Table 7, the total cost and energy cost of integrated model are also less than the separate  
35  
36 model by 4.1% and 8.0% respectively. The electricity procurement cost, material cost and  
37  
38 switching cost decrease by 99.5%, 0.2% and 53.5% respectively. But the inventory cost and coal  
39  
40 cost of integrated model are more than separate model. **Due to the low inventory cost, the**  
41  
42 **solution by the integrated model will prefer stabilizing the working state and production rate in**  
43  
44 **order to save energy. Inevitably, a higher inventory cost is resulted.**  
45  
46  
47

48 From case 1 and 2, the average decrease of total cost is 3.35% and the average decrease of  
49  
50 energy cost is 6.55%. So it is necessary to **propose an** integrated plant-wide material processing  
51  
52 system and utility system for planning optimization to acquire optimal benefit. It is clear that  
53  
54 changing demands affect the saving cost from the proposed integrated model comparing with the  
55  
56

separate model, and the cost saving quantity may be case specific. But the proposed integrated model method is superior to the separate model method.

**Table 6. Comparisons between integrated model and separate process model of case 1**

Items	Integrated model	Separate process model		
		Value(¥)	Difference	
			Absolute value (¥)	Relative value (%)
Total cost	166,392,500	170,889,508.8	4,497,009	2.6 ↓
Energy cost	79,406,633.5	83,641,810	4,235,176.5	5.1 ↓
Electricity procurement cost	3,456,700	7,053,810	3,597,110	51.0 ↓
Coal cost	75,949,933.5	76,588,000	638,066.5	0.8 ↓
Inventory cost	229,380	362,898.8	133,518.8	36.8 ↓
Material cost	86,712,386.5	86,847,000	134,613.5	0.2 ↓
Switching cost	44,100	37,800	6,300	16.7 ↑

**Table 7. Comparisons between integrated model and separate process model of case 2**

Items	Integrated model	Separate process model		
		Value(¥)	Difference	
			Absolute value (¥)	Relative value (%)
Total cost	154,813,500	161,467,526.8	6,654,026.8	4.1 ↓
Energy cost	75,830,099	82,456,290	6,626,191	8.0 ↓
Electricity procurement cost	61,049	12,271,720	12,210,671	99.5 ↓
Coal cost	75,769,050	70,184,570	5,584,480	8.0 ↑
Inventory cost	390,420	248,336.8	142,083.2	57.2 ↑
Material cost	78,551,681	78,674,000	122,319	0.2 ↓
Switching cost	41,300	88,900	47,600	53.5 ↓

## 6. CONCLUSION

This paper has addressed the integrated optimization of both plant-wide material processing

1  
2  
3 and utility system. An MINLP planning optimization model is proposed for a real-world PVC  
4  
5 plant in a discrete time period. The proposed model can reflect start-stop operation of several  
6  
7 energy-intensive processing units such as calcium carbide furnaces, electrolytic cells and CHP  
8  
9 units. Also, energy consumption has been taken into consideration by modeling the electricity  
10  
11 consumption characteristics of each calcium carbide furnace and electrolytic cell and by  
12  
13 modeling the coal consumption of each CHP unit. The optimal production distribution and  
14  
15 operation state of each type of equipment is proven to be instructive to a real-world PVC plant  
16  
17 planning optimization. Two cases originated from a real PVC plant have been provided to verify  
18  
19 the applicability of the proposed model. The comparisons between the integrated model and the  
20  
21 separate model show that about 3.35% of total cost and 6.55% of energy cost can be saved by  
22  
23 using the integrated model rather than the separate model. Large scales of proposed MINLP  
24  
25 model lead to long solution time and higher gap, then an efficient solving algorithm need to be  
26  
27 studied further.  
28  
29  
30  
31  
32  
33  
34  
35

## 36 ASSOCIATED CONTENT

### 37 Supporting Information

38  
39 Curves, functions and fitting accuracies of CHP units, calcium carbide furnaces and electrolytic  
40  
41 cells are shown in S1-S3 respectively. Parameters used in this case study are shown in S4.  
42  
43

44  
45 Production rate of calcium carbide furnaces and electrolytic cells of case 1 are shown in S5 and  
46  
47 S6 respectively.  
48

49  
50 This material is available free of charge via the Internet at <http://pubs.acs.org>.  
51  
52

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24  
25  
2627  
28  
29 NOMENCLATURE  
3031 **Indices**  
3233 i = product  
3435 r = raw material(coal, coke, lime, salt)  
3637 u = units (calcium carbide furnace/electrolytic cell/polymerization reactor/CHP unit)  
3839 w = time period  
40  
4142 **Sets**  
4344 E = electrolytic cells  
4546 EG = CHP units  
4748 FA = electrolytic cells, calcium carbide furnaces and CHP units  
4950 G = calcium carbide furnaces  
5152 M = polymerization reactors  
53  
54  
55  
56  
57  
58  
59  
60

1  
2  
3 MP = final products (grades of PVC)  
4

5 MR = raw materials(coal, coke, lime, salt)  
6

7 W = time periods  
8  
9

### 10 Parameters

11 CE<sub>w</sub> = price of electricity from the state grid

12 CI<sub>cac2</sub> = inventory cost of CaC<sub>2</sub>  
13

14 CI<sub>i</sub> = inventory cost of product i  
15

16 CI<sub>r</sub> = inventory cost of raw material r  
17

18 CI<sub>vcm</sub> = inventory cost of VCM  
19

20 CRM<sub>r</sub> = cost of raw material r  
21

22 CF<sub>u</sub> = cost of switching operation of unit u  
23

24 cy = polymerization time  
25

26 D<sub>i,w</sub> = market demand of product i in the period w  
27

28 FS<sub>u</sub> = feeding quantity of unit u  
29

30 MI<sub>cac2</sub><sup>max</sup> = maximum inventory capacity of CaC<sub>2</sub>  
31

32 MI<sub>cac2</sub><sup>min</sup> = minimum inventory capacity of CaC<sub>2</sub>  
33

34 MI<sub>i</sub><sup>max</sup> = maximum inventory capacity of product i  
35

36 MI<sub>i</sub><sup>min</sup> = minimum inventory capacity of product i  
37

38 MI<sub>r</sub><sup>min</sup> = minimum inventory capacity of raw material r  
39

40 MI<sub>r</sub><sup>max</sup> = maximum inventory capacity of raw material r  
41

42 MI<sub>vcm</sub><sup>max</sup> = maximum inventory capacity of VCM  
43

44 MI<sub>vcm</sub><sup>min</sup> = minimum inventory capacity of VCM  
45

46 P<sub>cac2,u,w</sub><sup>max</sup> = maximum production rate of unit u to produce CaC<sub>2</sub> in the period w  
47

48 P<sub>cac2,u,w</sub><sup>min</sup> = minimum production rate of unit u to produce CaC<sub>2</sub> in the period w  
49  
50  
51

1  
2  
3  $P_{cl2,u,w}^{max}$  = maximum production rate of unit u to produce  $Cl_2$  in the period w

4  
5  
6  $P_{cl2,u,w}^{min}$  = minimum production rate of unit u to produce  $Cl_2$  in the period w

7  
8  $P_{w,u,w}^{max}$  = maximum electric power of unit u in the period w

9  
10  $P_{w,u,w}^{min}$  = minimum electric power of unit u in the period w

11  
12  $P_{y_i}$  = stockout punishment of product i

13  
14  $T_{cl2}$  = processing time of an electrolytic cell during the period w

15  
16  $T_{cac2}$  = processing time of a calcium carbide furnace during the period w

17  
18  $T_{CHP}$  = processing time of a CHP unit during the period w

19  
20  $\alpha_{i,u}$  = conversion rate of VCM to product i in unit u

21  
22  $\beta$  = transfer coefficient for output of  $C_2H_2$  and consumption of  $CaC_2$

23  
24  $\gamma$  = transfer coefficient for output of HCL and consumption of  $Cl_2$

25  
26  $\delta$  = transfer coefficient for output of  $CaC_2$  and consumption of coke

27  
28  $\varepsilon$  = transfer coefficient for output of  $CaC_2$  and consumption of CaO

29  
30  $\epsilon$  = transfer coefficient for output of  $Cl_2$  and consumption of NaCl

### 31 32 33 34 **Variables**

35  
36  $CM_{cac2,w}$  = consumption of  $CaC_2$  in the period w

37  
38  $CM_{cao,w}$  = consumption of CaO in the period w

39  
40  $CM_{C_2H_2,w}$  = consumption of  $C_2H_2$  in the period w

41  
42  $CM_{cl2,w}$  = consumption of  $Cl_2$  in the period w

43  
44  $CM_{coal,w}$  = consumption of coal in the period w

45  
46  $CM_{coke,w}$  = consumption of coke in the period w

47  
48  $CM_{Hcl,w}$  = consumption of HCL in the period w

49  
50  $CM_{Nacl,w}$  = consumption of NaCl in the period w



1  
2  
3  $CM_{r,w}$  = consumption of raw material r in the period w  
4

5  $CM_{vcm,w}$  = consumption of VCM in the period w  
6

7  
8  $ele_w$  = electricity consumption of total PVC plant in the period w  
9

10  $elesp_w$  = electricity supply in the period w  
11

12  $MI_{cac2,w}$  = inventory of  $CaC_2$  in the period w  
13

14  $MI_{i,w}$  = inventory of product i in the period w  
15

16  
17  $MI_{r,w}$  = inventory of raw material r in the period w  
18

19  $MI_{vcm,w}$  = inventory of VCM in the period w  
20

21  $N_{i,u,w}$  = number of feeding batches in unit u to produce product i in the period w  
22

23  $P_{cac2,u,w}$  = production rate of  $CaC_2$  in unit u in the period w  
24

25  
26  $P_{cl2,u,w}$  = production rate of  $Cl_2$  in unit u in the period w  
27

28  $PE_{u,w}$  = electricity supply of unit u in the period w  
29

30  $PT_{cac2,w}$  = production of  $CaC_2$  in the period w  
31

32  $PT_{C_2H_2,w}$  = production of  $C_2H_2$  in the period w  
33

34  $PT_{cl2,w}$  = production of  $Cl_2$  in the period w  
35

36  
37  $PT_{i,u,w}$  = production of product i in unit u in the period w  
38

39  $PT_{vcm,w}$  = production of VCM in the period w  
40

41  
42  $Pw_{u,w}$  = power of unit u in the period w  
43

44  $S_{i,w}$  = supply of product i in the period w  
45

46  $SG_w$  = electricity supply of the state grid  
47

48  
49  $SP_{r,w}$  = supply of raw material r in the period w  
50

51  $Z_{u,w}$  = 0-1 variable denotes whether unit u is working in the period w  
52

53  $ZF_{u,w}$  = 0-1 variable denotes whether unit u starts up or shuts down in the period w  
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