Paper:

Andreoli, E. (2017). Materials and Processes for Carbon Dioxide Capture and Utilisation. *C - Journal of Carbon Research, 3*(2), 16

http://dx.doi.org/10.3390/c3020016

C Journal of Carbon Research

Editorial

Materials and Processes for Carbon Dioxide Capture and Utilisation

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Academic Editor: Craig E. Banks
Received: 3 May 2017; Accepted: 15 May 2017; Published: 19 May 2017

Materials and processes for CO_2 capture and utilisation are an essential part of a holistic approach toward a sustainable energy future. CO_2 and energy are tightly intertwined as energy produced from fossil fuel combustion always generates CO_2. A major environmental concern, CO_2 could also become an invaluable resource for making carbon-based materials and chemicals, and a means to store energy in CO_2-derived fuels. In this Special Issue of *C*, the reader can appreciate the complexity of the challenge from the perspective of energy production process engineering; materials science and chemistry; waste management; cross-disciplinary approach to policy and public engagement.

Electrical power generation from fossil fuels combustion is a major emitter of CO_2. Low carbon high quality power generation can be achieved using IGCC (Integrated Gasification Combined Cycle) technologies, where coal, for example, is converted to a gas mixture rich in H_2 and CO_2, with the latter captured before H_2 combustion. In such an IGCC power plant, hot H_2 combustion gasses drive a gas turbine, while heat from the coal gasifier is used to generate steam to drive a steam turbine, each coupled to a dedicated electric generator. Key to low carbon emissions is the pre-combustion capture process. In this Special Issue, Peampermpool et al. [1] at Curtin University show how 92% of CO_2 can be separated by means of a two-stage capture process consisting of (i) CO_2 cryogenic liquefaction, followed by (ii) expansion of resulting CO_2-lean gases through an orifice. Aspen HYSYS simulations of an energy-saving scheme specifically designed for this process indicate that the energy burden for CO_2 capture for a 740 MW IGCC GE power plant could be limited to 7.4–7.8%. It follows that process engineering can improve CO_2 capture technologies, as such carbon capture materials must also be improved as addressed in the next paragraph.

Novel materials for CO_2 capture are essential to decarbonise fossil-based energy production while transitioning to renewable-based energy generation. Very large amounts of CO_2 must be captured to be then used or stored. Efficient carbon capture materials are thus instrumental to CO_2 utilisation and storage. Porous carbon materials achieve high CO_2 capture capacities, while selectivity may be enhanced in the presence of chemical functional groups. Carbon foams with a large variety of functional groups can be prepared from H_2SO_4-dehydrated *para*-nitroaniline, as reported in the contribution of Andreoli and Barron [2]. Almost 35 atom % of surface nitrogen on these foams is amine and/or aromatic N, both known to enhance selective CO_2 adsorption. This is also confirmed by the value of heat of adsorption, 113.6 kJ/mol, in the range typical of amine-based chemical sorbents. In a related contribution, Ghosh and Barron [3] studied the role of Lewis base (LB) moieties including amines on CO_2 chemical sorption. The computational study shows how LB moieties alone cannot explain enhanced CO_2 capture via poly-CO_2 formation. For poly-CO_2 to be stable, Lewis acid (LA) moieties such as H^+, AlF_3, B_4O_6 should also be present to form LB-C(O)O-[C(O)O]n-C(O)O-LA species, where LA is bound to the negatively charged terminal oxygen.

Direct air capture (DAC) is the formidable challenge of capturing CO_2 directly from the Earth's atmosphere. The Glaser group at the University of Missouri-Columbia has specialised in the study and development of rubisco-inspired biomimetic approaches to the reversible capture of CO_2 from air. In their contribution [4], the group shows how the reversibility of CO_2 binding in a rubisco-based small molecule model is essentially dependent on a drop in entropy upon capture. While the overall Gibbs free energy change is negative, i.e., the capture is spontaneous, the decrease in entropy allows for an easy release of the CO_2 when the temperature is increased. The entropy drop is due to the two-tethered capture modality of rubisco: the freedom of movement of the two "clamping" arms (the Mg^{2+} centre and the lysine amino group) of the active site of rubisco is lost when CO_2 is inserted between the two arms to form carbamate with the amino group, and as the carbamate "clamps" on the Mg^{2+} centre via complexation that blocks the two arms in place with a corresponding large reduction of system entropy.

Other alternatives to carbon capture are possible by avoiding CO_2 emissions through the reuse or recycling of materials, a strategy to reduce greenhouse gases (GHG) emissions. CO_2 emissions can be avoided when manufacturing from recycled materials is less energy intensive than from virgin materials. Paper recycling can also result in additional forest carbon sequestration. However, as Lakhan states in his contribution to this Special Issue [5] "not all materials are created equal with respect to the environmental and economic benefits of recycling activity." Recycling electronic waste such as printers, computers, etc. can improve emissions offsets and reduce material management costs only for certain types of materials. For example, materials found in copying devices are better suited to recycling than those from display devices with a higher cost \$/tCO_2e (dollars spent on recycling activities required to reduce emissions by one tonne of carbon dioxide equivalent). Although these findings are specific for Ontario, the overarching message of "it is more important what, than how much" is recycled can be applied to other regions. This is particularly significant for policy planners now facing the challenge of how to achieve the goals of reducing GHG emissions.

Advancing low carbon technologies is not only a scientific and engineering challenge, but also the necessary opportunity for public participation from an early stage of development to deployment. Jones and Jones [6] present here a wonderfully written communication centred around the need to establish more effective collaborations between engineers and social scientists for new technologies to come to fruition. This is especially true for carbon dioxide utilisation (CDU), where a constructive contribution of the public to new environmental and energy solutions is strongly dependent on timely public engagement and communication. An outstanding example of embedded and sustained cross-cutting collaborative environment is the UK centre for CDU (CDUUK) at the University of Sheffield. At the CDUUK, carbon capture agents, life-cycle analysis of products and public perception are all addressed in concert, including providing a networking forum for CDU knowledge-exchange, the CO2Chem network [6].

In the future, CDU could allow for the integration of renewable energy generation within the existing energy infrastructure, as discussed in Rosa's thorough and overarching assessment of energy technologies [7]. CDU could provide the means to store intermittent renewable energy in synthetic hydrocarbon fuels made from CO_2 and H_2. The strength of this approach is the availability of storage for gaseous/liquid hydrocarbon fuels for both transportation and power generation. On a different but related note, CO_2 is also used for oil production through the so-called CO_2-mediated enhance oil recovery (CO_2-EOR). In CO_2-EOR, crude oil is made less viscous using supercritical CO_2 allowing further extraction from depleting reservoirs. Parallel to this process there is also the opportunity for CO_2 storage. To this end, it is relevant to monitor CO_2 emissions from CO_2-EOR sites. Chen and Roberts [8] contributed to the Special Issue with a study on the use of vegetation grow as a monitoring parameter of emissions CO_2-EOR sites. Findings suggest that with careful planning, vegetation monitoring could integrate other typical monitoring strategies such as formation pressure and air quality monitoring with the advantage of quantifying and modelling ecological effects. The remarkable diversity of aspects covered in this issue is evidence of the complex challenge ahead of scientists, engineers, regulators, and all other relevant stakeholders involved in implementing a sustainable energy future where carbon capture and utilisation technologies are to play a key role.

Conflicts of Interest: The author declares no conflict of interest.

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