

# Process Simulations and Experimental Studies of CO<sub>2</sub> Capture

José Ramón Fernández

Instituto Nacional de Ciencia y Tecnología del Carbono, Spanish Research Council (INCAR-CSIC), Francisco Pintado Fe, 26, 33011 Oviedo, Spain; jramon@incar.csic.es; Tel.: +34-985119090

Carbon dioxide, whose global emissions into the atmosphere have reached a maximum of about 36 billion tons per year (compared to the 6 billion tons emitted in 1950), is considered by far the main greenhouse gas (GHG) [1]. The net greenhouse gas emissions need to become zero or even negative beyond 2050 to comply with the Paris Agreement and keep global warming well-below 1.5–2 °C with respect to pre-industrial levels [2]. Significant progress has already been made in reducing the energy intensity and the carbon footprint in industrial processes, but this effort must be accompanied by the definitive deployment of CO<sub>2</sub> capture and permanent storage (CCS). CCS is a chain of processes from the CO<sub>2</sub> capture to its transport and long-lived storage, with CO<sub>2</sub> capture being the most expensive and energy-intensive step [1]. CCS requires still a great rate of deployment to meet the targets for the mitigation of climate change, as currently less than 40 million tons of CO<sub>2</sub> are captured and finally storage [3].

Three routes have been identified as CO<sub>2</sub> capture strategies: post-combustion, pre-combustion, and oxy-combustion. The post-combustion technologies remove the CO<sub>2</sub> from flue gases at relatively low CO<sub>2</sub> partial pressure (typically containing between 10 and 15% of CO<sub>2</sub>). Post-combustion is considered an end-of-pipe solution, which may be integrated into existing processes with reasonable low alterations in the plant layout. However, its efficiency is limited in industries with multiple CO<sub>2</sub> emission points (boilers, furnaces, etc.), as happens in steel manufacture plants and the petroleum refining industry (both responsible of about 12% of carbon emissions worldwide) [4]. In pre-combustion systems, carbon is present in the form of CO and CO<sub>2</sub> resulting from previous steam reforming or gasification processes. Then, this carbon is totally converted into CO<sub>2</sub> and subsequently separated from hydrogen at high pressure. The production of low-carbon hydrogen has attracted great interest over the last years to be used as clean source of energy or as feedstock for the production of ammonia, methanol or synthetic fuels (mainly via Fischer–Tropsch) as a sustainable way to substantially reduce the carbon footprint of these industries [5]. Finally, in the oxy-combustion systems, the combustion of the fuel takes place with pure oxygen rather than air, giving as a result a virtually pure CO<sub>2</sub> stream due to the absence of nitrogen in the incoming comburent gas. However, to maintain CO<sub>2</sub> purity any potential air infiltration in the system must be avoided, which implies rigorous and costly safety procedures.

This Special Issue compiles the successful submissions about innovative investigations elaborated by prominent researchers from different disciplines, which will provide a substantial advance in the state-of-the-art in the field of the CO<sub>2</sub> capture and storage technologies. The most relevant features of the main research lines and the findings presented by the contributions to this Special Issue are summarized below.

The vast majority of large-pilot and commercial CO<sub>2</sub> capture, transport, and storage plants have been so far launched in developed countries. This is due to the fact that the main efforts aimed at implementing policies and regulatory frameworks to spread CCS have been put into effect in the developed world [6]. However, it is expected that energy demand grows strongly in the developing countries in coming decades, and therefore, about 70% of CCS development should be carried out in these regions in order to meet the long-term



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climate targets included in the 1.5–2 °C global emission scenario [2]. Therefore, progress in CCS deployment must be accelerated in developing countries. Rich nations need to provide developing regions with not only financial support to facilitate the transition to low-carbon economy but also the experience gained in successful large-scale operating projects to reduce costs and risks in future scaling up of CCS technologies in the developing countries.

Fragkos [7] shows strong evidence of the potential role of carbon capture and storage for the decarbonisation of developing regions when it is integrated in power generation and industrial processes. The author uses an advanced version of the PROMETHEUS energy model, in which the socio-economic impacts of COVID-19 pandemic are considered. This model provides foresights about challenges and also opportunities for the deployment of CCS technologies in developing regions, especially in those where the expansion of renewable energy and nuclear power are limited. The study reveals that the low implementation of CCS in developing economies demands additional funding focused on bringing down CO<sub>2</sub> capture costs together with new climate policies that consider subsidies for low-carbon investigation, tax credits, or regulatory support for CO<sub>2</sub> grids.

Amine scrubbing is the most mature CO<sub>2</sub> capture technology to date. Although the absorption with amines was initially proposed to separate acidic gases from gaseous mixtures, over the last decades, this process has been studied in detail for the particular application in CO<sub>2</sub> removal [8]. In this process, the flue gas enters the absorption unit and flows from the bottom upwards being put into contact with a counter-current stream of lean solution. CO<sub>2</sub> is then absorbed and the flue gas free of CO<sub>2</sub> leaves the top of the absorber. The loaded solution is directed to the top of a stripper column to carry out the regeneration of the solvent at higher temperature. The solution flows down against a counter-current flow of steam, and most of the CO<sub>2</sub> is removed from the solvent. Once the mixture of CO<sub>2</sub> and steam leaves the stripper, it is circulated through a condenser where steam is condensed. Subsequently, it enters a reboiler and returned returns to the system, while pure CO<sub>2</sub> is obtained. Meanwhile, the lean solution is cooled down and pumped back to the absorber. Monoethanolamine (MEA) or methyl diethanolamine (MDEA) are the most common solvents used in amine scrubbing. More advanced materials, such as diethanolamine (DPA), dominoethoxyethanol (DGA), piperazine (PZ), diisopropanolamine (DIPA), or triethanolamine (TEA) are also being developed in order to overcome an important number of operating issues found during the scaling of this technology. These issues include solvent degradation at high temperatures, the generation of hazardous waste sub-products resulting from this degradation, the high cost of solvent production, the limited concentration of the solvent allowed to avoid corrosion, adverse reactions with minority components in the flue gas (e.g., SO<sub>2</sub>, oxygen, etc.), and high energy penalty in the sorbent regeneration stage (involving energy penalty up to 12%).

Aromada et al. [9] evaluate different designs of heat exchangers (HX) used as lean/rich HX in amine-based CO<sub>2</sub> capture processes with the purpose of reducing the equipment costs (CAPEX) of this technology. In contrast with typical shell and tube heat exchangers (STHX), there are other configurations with potential use in this type of absorption processes, such as finned double-pipe (FDP-HX), gasketed-plate (G-PHE), or welded-plate (W-PHE). Once the technical strength and limitations of the above-mentioned heat exchangers have been assessed, it is concluded that gasketed-plate HX is the most economical option, as reductions of CO<sub>2</sub> capture costs of 5–6 EUR/tCO<sub>2</sub> are feasible if G-PHE are used instead of more conventional STHX, giving rise to moderate overall costs of around 60 EUR/tCO<sub>2</sub> for the entire amine-based CO<sub>2</sub> capture process.

The modification of microporous materials, such as zeolites, silicates, activated carbons, or metal-organic frameworks (MOFs), via the loading of amines is a well-known technique to obtain advanced solid chemisorbents. Sánchez-Vicente et al. [10] have developed a novel adsorbent-based material (diamine-SBA-15) by functionalizing a silica-based solid using an amine compound in supercritical CO<sub>2</sub> modified with methanol or ethanol. The objective is to obtain a hybrid CO<sub>2</sub> adsorbent, which is able to perform in wider operating conditions, requires less energy for regeneration, reduces amine corrosivity, and generates safer solid

waste. It has been found that diamine-SBA-15 shows high surface area and pore volume, which allows maximum CO<sub>2</sub> capture capacities near 1 mmol CO<sub>2</sub>/g at ambient conditions. These results show that this silica-based material loaded with amine is a promising CO<sub>2</sub> capture sorbent for post-combustion processes or direct air capture.

Cai et al. [11] have investigated numerically and experimentally the use of supercritical CO<sub>2</sub> to obtain shale gas. The results show that supercritical CO<sub>2</sub> jet fracturing is a more sustainable method compared to that using water for rock breaking, as the consumptions of water and energy are substantially reduced. A numerical method to analyse the flow field of the supercritical CO<sub>2</sub> jet fracturing has been developed, which has been successfully validated with experimental results. The proposed model allows the evaluation of different factors, such as the dimensions of the nozzle or the aperture ratio on flow field and on flow characteristics (e.g., velocity distribution) of supercritical CO<sub>2</sub> jet fracturing. A high-speed photography technique (HSP) has been used to monitor the perforation during experiments.

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