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Can we systematically rank the performance of any existing material for sorbent-based carbon capture?

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Abstract

Since the Paris agreement in 2015 and the more recent release of the IPCC report in 2018[1], more global efforts are driven to reverse climate change, particularly reducing, eliminating, and removing greenhouse gases before being released into the atmosphere. Countries are being challenged to come forward with ambitious 2030 emissions reduction targets for reaching net-zero by 2050 and keep 1.5 degrees within reach by 2100. In the COP26 summit, 26 nations gathered to finalize the Paris Rulebook and accelerate action to tackle the climate crisis. However, achieving net-zero is not an easy task as there are sectors that are more challenging to decarbonize.

With our work, we aim to accelerate the pace of development for the decarbonization of the power and industrial sectors by ultimately providing cost-effective solutions for carbon capture applications. For this, we evaluated the performance of thousands of adsorbents in sorbent-based carbon capture processes.[2–3] To achieve this, we bridge molecular simulations with process modelling. Molecular simulations are used to predict the pure component isotherms of a library containing the crystal structure of thousands of potential adsorbents. These simulated isotherms are the input to the process model, from which we obtain a material ranking and process performance evaluation (see Fig. 1), and we provide a set of optimal structures for each application (illustrated in Fig. 1 as case study characteristics). In our ranking, we consider the characteristics of the source of CO_2 (e.g., industrial plants, power plants, direct air capture, etc.) and the sink/destination of the CO_2 (e.g., geological storage, mineralization, etc.).

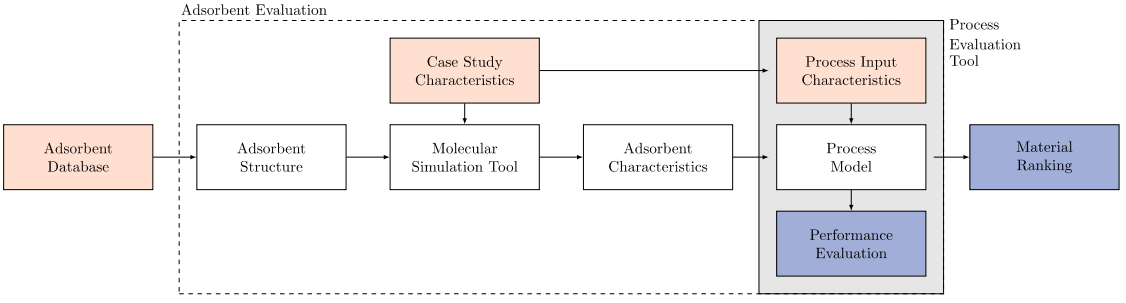

Fig. 1 | The workflow. A schematic depiction of our workflow that we used to evaluate the performance of thousands of structures in a specific carbon capture technology and for a specific application. The input data are highlighted with a light orange color and the output blue.

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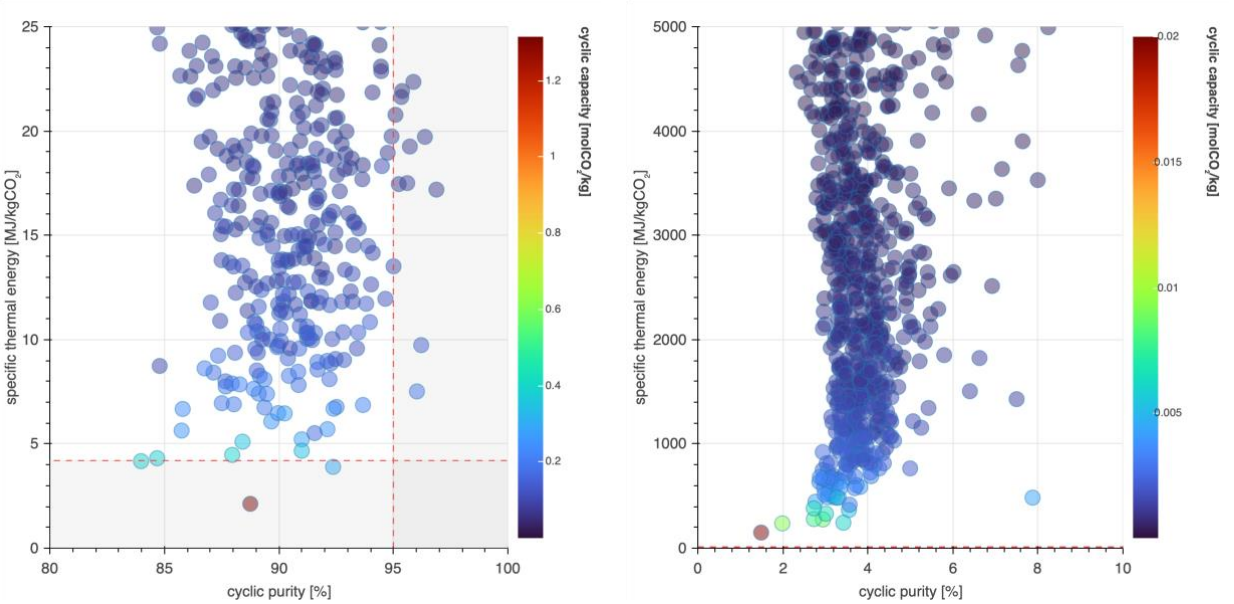
In this study, we selected two different case studies to demonstrate how we rank materials for a particular application, including different CO_2 concentrations in the feed stream and different CO_2 destination, i.e., carbon capture from a natural gas (NG) offshore power plant where the CO_2 is sent for geological storage, and direct air capture (DAC) for supplying CO_2 to greenhouses. First, we computed the physicochemical and adsorptive properties of 1284 metal-organic frameworks (MOFs) available in the CoRE MOF database[4] using various computational techniques.[5] Next, we evaluated the performance of these structures using an in-house temperature vacuum swing adsorption (TVSA) model and assuming a binary mixture of CO_2 and N_2. More details on our workflow can be found in [6,7]. The main process characteristics for each case study are summarized in the caption of Fig. 2.



(a) NG offshore case study (b) DAC case study

Fig 2. | Ranking results of 1284 structures using a TVSA process for (a) carbon capture from NG offshore and for geological storage and (b) DAC for plant enhancement in greenhouses. The plots show the specific thermal energy requirements, which include the total sensible heat and heat of adsorption, versus the purity. The colors correspond to the cyclic capacity of the process which is the amount of the collected CO_2 product per kg of adsorbent. The TVSA process is a four-step process that consists of adsorption, vacuum, open heating, and open cooling (+pressurization) steps. The input parameters are: (a) 3.68% CO_2 in the inlet stream, 30°C adsorption temperature, 100°C desorption temperature, and vacuum at 0.01 bar. (b) 0.04% CO_2 in the inlet stream, 10°C adsorption temperature, 100°C desorption temperature, and vacuum at 0.01 bar.

Fig. 2 illustrates the material ranking for both selected applications. For application (a) NG offshore, the targeted CO_2 purity was set >95% and the specific energy demand was set <4.2 MJ/kgCO_2 to be competitive with conventional carbon capture processes.[8] For application (b) DAC, the target is to purify the CO_2 without setting a constraint but to achieve energy requirements below 11.9 MJ/kgCO_2 (values achieved in DAC systems reported in the literature).[9,10] Fig. 2(a) shows that for the NG offshore case study there are some structures that can meet the purity constraint and some others that can meet the energy constraint (although the electrical energy is not included in this plot). However, in this standard and non-optimized TVSA process, we were not able to locate structures that can meet both requirements. Fig. 2(b) shows that for the DAC case study the assumed 4-step TVSA process and the selected 1284 structures cannot meet the requirements of an efficient separation process. Further work is needed for identifying structures that can meet the purity and energy criteria.

In this study, we present a workflow that allows for ranking hundreds of structures for different carbon capture applications. In the short future, more structures will be added to the workflow and the materials space will be further explored. We will also screen for different process configurations and under optimal process parameters, which can be obtained by applying process optimization. Finally, we are currently expanding the performance indicators (e.g., purity and energy consumption) to include economic and environmental indicators as part of the integration of techno-economic assessment (TEA) and life cycle assessment (LCA) models. Our ultimate task is to link materials to processes for several carbon capture sources and destinations for the fast-track development of sorbent-based carbon capture.

Keywords: carbon capture; material screening; process integration; molecular simulations; adsorption

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