

Research Projects for graduate students at the Center for Negative Carbon Emissions

Background:

A central activity of the Center for Negative Carbon Emissions is the demonstration of direct air capture technologies with machinery that can operate in open environments. Initially a major focus of the Center is on demonstrating air capture based on the humidity swing. However, work at the Center over time will consider other approaches as well. The demonstration requires a large engineering effort that is supported by a basic science approach and a general modeling and assessment effort.

Demonstration can range from a proof of principle of a new method to the complete development of a practical system operating at a significant scale in an outdoor environment. Demonstrations will initially focus on delivering carbon dioxide in more or less concentrated and pure form, but the carbon dioxide produced will also be further processed for specific applications and uses of carbon dioxide. Carbon dioxide can be recovered as a component of a sweep gas like air, as pure concentrated and pressurized carbon dioxide, or as CO₂ or bicarbonate dissolved in water. CO₂ can be transformed into solid carbonates for disposal, or used as feedstock for the production of synthetic fuels. The design of the product stream of captured CO₂ will be informed by the demands and requirements of the application. Applications may pose specific requirements concerning the physical state of the CO₂, the associated impurities and/or carriers. Applications also can pose challenges by returning sweep-gases or carrier materials contaminated with impurities picked up in the interaction with the downstream process.

Demonstrations will be supported by detailed modeling and assessment of the technology, with modeling efforts ranging from the molecular scale, to continuum models that characterize transport in simple components of the system, modeling at the device level and ultimately at the full system scale. On the system scale, the integration of techno-economic assessments transcends simple engineering and physical modeling. Indeed, TEA will extend toward TESPEA (Techno-Economic-Socio-Political-Environmental Assessments) of the concept.

Scientific modeling will go hand-in-hand with fundamental science in support of air capture technology. Again this will range from understanding the mechanism underlying the current sorption process, the extension of this process to novel materials, the rebuilding of the process on device scale, and the engineering science that goes into making design decisions. On the latter point we have argued that the construction of many small systems that can – in a modular fashion—be integrated into one large infrastructure. Understanding the scaling laws that govern these kinds of technologies is therefore crucial.

Graduate students interested in a Ph. D. project can take ownership of many different aspects of the project. There is an immediate need to develop a first prototype that can produce carbon dioxide enriched air. A student involved will contribute directly to the design of the apparatus, of the testing protocol and the specification of what such a machine needs to be able to deliver. Individual students may pursue the system development or aspects of the system development or take ownership of a particular subsystem. Others may focus more on the modeling effort, where new ideas are needed at virtually every scale.

The following are a set of specific projects in need of a champion. These projects as described are topics the Center for Negative Emissions will work on and develop. They contain the beginnings of thesis projects but they will have to be tailored to meet specific research interests and adjust to particular backgrounds and skills of a student. Projects can be combined or broken up into several projects. Thesis projects would derive from these concepts and focus on specific aspects that can be more easily converted into academic papers.

1. **Design of physical structures to passively collect CO₂ from air.** This project will require a fluid dynamic analysis of a structure that is optimized for contacting air so that CO₂ can be transferred to sorbent surfaces. The project may deliver several different geometries optimized for different situations, and help in rationalizing the future design for prototype units at CNCE. Depending on the skills and interests of the student, this project could incorporate the construction of prototypes or leave this to a separate project. The performance of the prototype machine will be used to benchmark the model. The project should deliver a first design in short order, but could go on to advance the concept of a contactor in various ways: (a) optimize contact with the sorbent at minimum pressure drop, allowing for design constraints due to the specific characteristics of the sorbent material; (b) develop different options for regeneration in conjunction with research that determines what physical limits are imposed on the transport in and out of the sorbent material; (c) design structures that are capable of withstanding high winds (and other physical impacts in an open environment). An outcome of such a thesis might be a comprehensive understanding of open air scrubbers that could for example consider biologically inspired structures (e.g. trees that bend in the wind and naturally orient leaves to maximize their exposure to sunlight and or the transport of material to and from the leaf). This study could also address a scaling analysis.
2. **Design and automation of a regeneration system.** Design and development of a regeneration system is followed by the development of an automated system. The thesis project would have to establish a basic regeneration design of the sorbent material, and then optimize the system allowing for variations in environmental conditions. This would require a chemical engineering approach to developing a regeneration scheme, but it would also have to develop control algorithms that can adapt to different environmental conditions. The project should identify common themes in automation and to develop sensor technologies to make decisions. For example, it has been hypothesized that the loading state of the resin will have a direct impact on the infrared absorption characteristics of the resin. If this indeed the case, then it would be possible to design an infrared analyzer to estimate the state of CO₂ loading of a resin and thereby help in optimizing the loading cycle.
3. **Scaling studies in air capture and other technologies.** This project not only deals with physical scaling but also the techno-economic and socio-political implications of being able to start small and build out a modular massively parallel system. Technical questions involve building prototypes and reach an automation level that actually makes it work. Economic questions look at the implication of learning curves on future costs. (These kind of studies could be broader than just air capture). The advantages of starting small and the comparison to developing large point source capture will be explored, analyzed and used in developing strategies for introducing air capture technology.

4. **CO₂ compression system.** Develop a small scale compression system. Most compressors are designed to operate on large gas flows. Compressors aiming to process a tens of grams per second are generally considered too small to benefit from economies of scale. However, we envision the design and construction of many such units that operate in parallel, but they are too far apart to benefit from a single large compressor. We are developing a thesis project that would look at CO₂ compressors that can naturally operate at small scale.
5. **CO₂ and liquid air based compression.** One specific approach to small scale compression of CO₂ recovered from air is to freeze solid CO₂ out a gas stream. One potential working fluid for such a system could be air that is liquefied when renewable energy is available and removed. Not only does the cooling concentrate the CO₂ to high densities that under warming translates into high pressure, but also such a system will result in highly purified CO₂ as it is possible to remove all impurities like water that condense or freeze out at much higher temperatures, and avoid the accumulation of low condensation gases like nitrogen, oxygen and argon, which at CO₂ sublimation temperatures are still well above the boiling points of their liquid phases. This project could consider alternative cooling fluids to air, and it could develop systems designs for using cryogenics as an intermediate energy storage system. Lessons learned in this context could easily apply to other carbon management strategies
6. **Ocean liming.** We aim to understand the potential for capturing carbon dioxide from the air, use the resulting carbonic acid to dissolve lime stone into seawater that subsequently is allowed to dilute itself into the seawater. We aim to demonstrate this particular method of air capture, show how it could be implemented on a large scale and also analyze the efficacy and environmental safety of this approach to carbon management.
7. **Alternative sorbents.** The sorbents that so far have been explored are all of a family of polystyrenes functionalized with quaternary ammonium ions. However, we have experimental data suggesting that activated carbon impregnated with alkali hydroxide solutions is not only a good sorbent for CO₂, but also in contrast to its constituents, displays a clear moisture swing sensitivity. This suggests that the effect we are looking for is not limited to a particular class of resins, but could also be implemented in other sorbents. A more systematic search of alternative sorbents could start with an experimental program in search of such materials, with molecular dynamics calculations looking for mechanisms that could be found in a broader class.
8. **Techno-economic assessments and life cycle assessment.** There are a number of projects relating to the techno-economic assessment and life cycle assessment of this technology. Projects range from modeling the technology to considering the carbon footprint of the technology, to determining practical limitations to the technology.