Opportunity Notice for Partners to Assist NETL in Adapting CCSI Tool Set

Background

A large amount of the research and development of post-combustion carbon capture technology focuses on three main technologies: adsorption, absorption and membranes. Each of these technologies have energy and techno-economic advantages and disadvantages. However, an optimal process may involve the integration of multiple technologies into a single, hybrid, transformative process that is more economical and energy efficient. The challenge of developing this type of process is the integration of rigorous process sub-models into a single framework, where hybrid designs can be evaluated and optimized.

The National Energy Technology Laboratory (NETL) has significant expertise in the development of rigorous process models and modeling for the advancement and acceleration of the commercialization of carbon capture process systems. A large part of the effort is the Carbon Capture Simulation Initiative (CCSI) [Reference 1]. The computational tools and multi-scale modeling techniques comprising the CCSI Toolset can be broadly applied for the development of a wide variety of technologies well beyond carbon capture including chemicals production, petroleum refining, natural gas processing and biofuel production.

Need

NETL is seeking to undertake the development of rigorous process sub-models for the previously mentioned technologies and a framework for integrating them so that a hybrid, post-combustion CO_2 capture process applied to the flue gas of a typical Once-Through Steam Generator (OTSG) can be developed. To complement its existing expertise and capabilities, NETL is seeking one or more partners who can assist in the following Tasks:

Task 1. Models for amine scrubbing

This task has two sub-tasks:

> Subtask 1a: Develop a representative flowsheet model in Aspen Plus for aqueous piperazine
> This subtask will focus on development of a representative flowsheet for a process using aqueous piperazine scrubbing for CO_2 capture that will be developed and converged in Aspen Plus. The overall process model shall be developed and validated in such a way that the thermodynamic and kinetic sub-models accurately represent the response of the solvent over the range of conditions that may be encountered in commercial operation. Other solvents may be considered at the same level of detail as funding permits and pending adequate data availability; applicants should provide background on their ability to and successes in modeling other solvent systems. Models for all solvents will require a rigorously developed property model that has been validated separately from the overall process model. For additional information on expected data requirements and validation, please refer to CCSI's MEA model in Reference 2.
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> Subtask 1b: Prepare model for hybrid flowsheet design for integration into an Aspen Plus Model
> After the solvent model in Subtask 1a is converged, it will be used as the basis to develop a reasonable design for the hybrid configuration. A hybrid model may present opportunities for improved operation, but also may result in the amine scrubbing processes operating in different operating regions than a typical, optimized, single technology flowsheet. This subtask is designed to ensure that the model is built in a rigorous and fundamental manner such that material through system representation is accurate across the wide range of operating conditions and process configurations that may be encountered in practical operation. The applicant shall

propose a method for ensuring the solvent model is robust to changes in operating conditions that may result from hybrid operation. In the context of a solvent-membrane hybrid system, the proposed method shall also include anticipation of potential operating conditions over which the solvent model should operate reliably.

The estimated time to complete Task 1 is nine (9) months.

Task 2. Membrane Model

This task will consist of the completion and validation of a membrane model in ACM or similar. A detailed description of this task follows.

NETL will provide a model for membrane based CO_2 capture which will include rigorous treatment of membrane transport properties and different membrane configurations including hollow fiber and flat sheet type membranes. The models will consider mass transfer properties such as selectivity and gas permeance of the membrane, and consider temperature and concentration dependence. In addition, due to the large amount of gas flow rates in typical CO_2 capture applications, the membrane will attempt a rigorous accounting of the pressure drop due to effects from the permeate and flow configurations. The final version of the model will be generic and will provide default values of the parameters that can be easily overwritten by the user. The applicant shall propose a method to ensure that the membrane model will be robust enough for integration with task 1, allowing for the model's inclusion into the hybrid configuration development efforts. The applicant will also provide guidance on the representation of transport properties and commercially important flow configurations.

The estimated time to complete this task is twelve (12) months.

Requirements/Qualifications
To develop the solvent-hybrid carbon capture model, NETL is seeking a research team with the following expertise:

• Extensive modeling expertise in developing rigorous, high-fidelity, first-principle models for absorption post-combustion CO_2 capture systems. The applicant should have extensive experience in developing submodels for aqueous piperazine solvents processes, including thermodynamic and kinetic, heat and mass transfer, and hydrodynamic submodels. These submodels should be validated with experimental data over the entire range of operating conditions that can be encountered in a commercial process. In addition, the applicant should have experience in constructing Aspen flowsheets for absorption post-combustion systems, preferably with combing multiple carbon capture technologies into a single process.

To develop the membrane based carbon capture model, NETL is seeking a research team with the following expertise:

• Extensive modeling expertise in developing rigorous, high-fidelity, first-principle models for membrane post-combustion CO_2 capture systems. The applicant should have extensive experience in developing membrane models with rigorous membrane transport properties with different membrane configurations including hollow fiber and flat sheet type membranes. The applicant should have experience in process modeling in Aspen Plus, Aspen Custom Modeler, MATLAB, or similar platforms and experience in CFD membrane model development is a plus.

Instructions
Each submittal shall include the following: a) Cover Page that identifies the entity name, address, and point of contact information; b) Technical Discussion (not to exceed four (4) pages), which addresses the requirements and qualifications identified above as well as the evaluation criteria identified below including key personnel contributions and facilities and equipment; and c) Budget Page summarizing the labor categories (PI, post-doc, student, research fellow etc.), level of effort for each labor category, supplies and materials and overall proposed project cost.

Please limit responses to a maximum of six (6) pages of text, single spaced, 11-point font, with 1-inch margins. Illustrations, maps, figures, and tables may be used to supplement your response; the maximum length of your response including illustrations, maps, figures, and tables is nine (9) pages. Responses must be provided as a PDF attachment to the email, not to exceed 10 MB in size.

Responses Due Date
Responses to this Opportunity Notice are due no later than 8:00 AM EDT June 21, 2017. Responses are to be submitted electronically in Adobe Acrobat PDF to the National Energy Technology Laboratory (NETL) at the following e-mail address: CCSIToolsforOTSG@netl.doe.gov. Proposers can expect to receive a response from NETL by four weeks past the submission date.

Evaluation Criteria
Submittals will be evaluated on the following criteria:

(1) Overall technical understanding and merit;
(2) Qualifications and experience of proposed key personnel including organizational and management experience;
(3) Adequacy of proposer's site, facilities, capabilities and equipment; and
(4) Adequacy and feasibility (reasonableness) of the proposed approach.

Each criterion will carry equal weight. The selection decision will be based on overall best value.

Contacts
For questions regarding this Opportunity Notice, please to contact NETL at CCSIToolsforOTSG@netl.doe.gov.

Administration by Federal and Non-Federal Personnel: When considering responses to this Opportunity Notice, Federal employees are subject to the non-disclosure requirements of a criminal statute, the Trade Secrets Act, 18 USC 1905; the Government may also seek the advice of qualified non-Federal personnel. The Government may also use non-Federal personnel to conduct routine, nondiscretionary administrative activities. The respondents, by submitting their response, consent to DOE providing their response to non-Federal parties. Non-Federal parties given access to responses must be subject to an appropriate obligation of confidentiality prior to being given the access. Submissions may be reviewed by support contractors and private consultants.

References

1. CCSI and Toolset https://www.netl.doe.gov/research/coal/crosscutting/carbon-capture-simulation-initiative
2. Chinen, A. S., Morgan, J. C., Omell, B. P., Bhattacharyya, D., & Miller, D. C. (2016). Dynamic Data Reconciliation and Model Validation of a MEA-Based CO 2 Capture System using Pilot Plant Data. IFAC-PapersOnLine, 49(7), 639-644.