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Predicting the performance uncertainty of a 1-MW pilot-scale carbon capture system after hierarchical laboratory-scale calibration and validation

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ABSTRACT

A challenging problem in designing pilot-scale carbon capture systems is to predict, with uncertainty, the adsorber performance and capture efficiency under various operating conditions where no direct experimental data exist. Motivated by this challenge, we previously proposed a hierarchical framework in which relevant parameters of physical models were sequentially calibrated from different laboratory-scale carbon capture unit (C2U) experiments. Specifically, three models of increasing complexity were identified based on the fundamental physical and chemical processes of the sorbent-based carbon capture technology. Results from the corresponding laboratory experiments were used to statistically calibrate the physical model parameters while quantifying some of their inherent uncertainty. The parameter distributions obtained from laboratory-scale C2U calibration runs are used in this study to facilitate prediction at a larger scale where no corresponding experimental results are available. In this paper, we first describe the multiphase reactive flow model for a sorbent-based 1-MW carbon capture system then analyze results from an ensemble of simulations with the upscaled model. The simulation results are used to quantify uncertainty regarding the design's predicted efficiency in carbon capture. In particular, we determine the minimum gas flow rate necessary to achieve 90% capture efficiency with 95% confidence.
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1. Introduction

Flue gas produced during coal combustion at coal-fired power plants contains a large amount of carbon dioxide (CO_2) and, when directly released to the atmosphere, is a major contributor to global climate change. Carbon capture and sequestration can be an effective way to reduce the amount of CO_2 emissions and form part of a strategy to stabilize global climate change. As stated in [1], "achieving substantial reductions in temperatures relative to the coal-based systems will depend on rapid and massive deployment of some mix of conservation, wind, solar, and nuclear, and possibly carbon capture and storage." However, it is well recognized that current carbon capture and storage technologies must improve and mature before contributing to any significant portion of the mitigation portfolio. In practical terms, technological improvements during scale up are vital for commercial viability within the power generation sector [2,3]. To accelerate development and deployment of post-combustion carbon capture technology, the Carbon Capture Simulation Initiative (CCSI), a partnership between U.S. Department of Energy (DOE) national laboratories, industry, and universities, was created to improve the state-of-the-art computational modeling and simulation tools employed for efficient carbon capture [4].

Much research has been devoted to developing carbon capture technology that minimizes the energy penalty to coal-fired power plants [5]. As an alternative to amine-based aqueous solvents that require high energy costs for regeneration, scientists at the National Energy Technology Laboratory (NETL) have developed amine-based solid sorbents [6] to capture CO_2 from flue gas with a reduced energy penalty, minimal water use, negligible corrosion, and fewer operational issues [7]. Most of the work involving solid sorbents contributes to the development of the sorbent itself, while only limited studies focus on the design of an entire reactor system using computational tools. Recently, a computational fluid dynamics (CFD) model was developed in FLUENT to explore the innovative reactor design using a rotating fixed bed [8]. In the past, several modeling studies have evaluated small-scale solid sorbent adsorber performance [9] using a single CFD model, as well as CFD models developed in FLUENT and BARRACUDA [10], where the strengths and weaknesses of different CFD models are explored for the same small-scale reactor design. However, few studies have addressed

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the challenging problem to predict, with uncertainty, pilot-scale adsorber performance with no existing direct experimental data, which is the focus of this paper.

Solid sorbent-based capture systems are inherently complex and involve complicated multiphase, multiphysics, and multiscale phenomena. In CCSI, high-fidelity CFD models for multiphase reactive flow have been developed to simulate the complex physical and chemical processes of sorbent-based carbon capture and gain more insights on flow field and reaction behaviors in reactors using the open-source Multiphase Flow with Interphase eXchanges (MFIX) (https://mfix.netl.doe.gov) code. Although MFIX has been independently verified for various simple and small-scale multiphase reactive flow problems [11–13], rigorous model validation with quantified confidence on quantities of interest must be performed when such simulations are executed at the pilot scale and the results subsequently are used to inform system-level designs and decision-making. Because it is not currently feasible to conduct a direct model validation for the 1-MW (MW) pilot-scale carbon capture system due to the lack of experimental data at that scale, the MFIX-based CFD predictions must be progressively validated and calibrated so the predictive confidence at scale can be quantitatively characterized through statistical-based uncertainty propagation.

To accomplish this, CCSI has developed a hierarchical calibration and validation framework for solid sorbent-based capture (Fig. 1) [14,15]. Starting from the very bottom layer in Fig. 1, the complex physics and chemical processes of carbon capture are first decoupled into several unit problems with increasing levels of complexity. Each unit problem represents a unique model component that targets individual physics, including hydrodynamics, heat transfer, and chemical reactions.

A laboratory-scale carbon capture unit (C2U), built at NETL (shown on the experiment side in Fig. 1), provides the experimental data for hierarchical model validation, and a batch of experiments has been carried out with various control parameters to reproduce the unit problems. More details about the C2U experiment design and results can be found in our previous study on the hierarchical calibration and validation of carbon capture models for C2Us [16]. The entire validation process includes step-by-step model validation with increasing model complexity by introducing new physics and governing equations with associated model parameters into the previously validated and calibrated models. Beginning with cold non-reacting flow to hot non-reacting flow and subsequently to hot reacting flow with chemical reactions, a series of parallel C2U experiments have been conducted to provide data for model parameter calibration at each step of the C2U model validation hierarchy. A Bayesian calibration procedure, where the posterior distributions of model parameters obtained at each unit-problem level are used as prior distributions for the same parameter set in the next level of the unit problem, is employed.

Following this validation hierarchy, model parameters critical to carbon capture prediction have been identified and calibrated [1]. The posterior distributions of these parameters based on Bayesian calibration now will enable at-scale prediction for the pilot-scale design with a predictive confidence interval. This paper focuses on applying the validated and calibrated multiphase reactive models at the laboratory scale to quantify the prediction confidence for the conceptual 1-MW pilot-scale carbon capture design (the shaded elliptic box in Fig. 1).

The paper is organized as follows: Section 2 describes the conceptual design of the 1-MW pilot-scale adsorber with geometry, dimension, and typical operating conditions. The corresponding CFD models for the 1-MW pilot-scale adsorber are presented in Section 3. Section 4 introduces the nominal settings for the simulations and statistical data analysis that result in a confidence interval for the at-scale predictions. The paper concludes with Section 5.

2. MW pilot-scale adsorber conceptual design

2.1. Adsorber geometry and operation conditions

Typical pilot-scale CO_2 capture systems consist of two main components: 1) the bubbling bed adsorber and 2) moving bed regenerator.

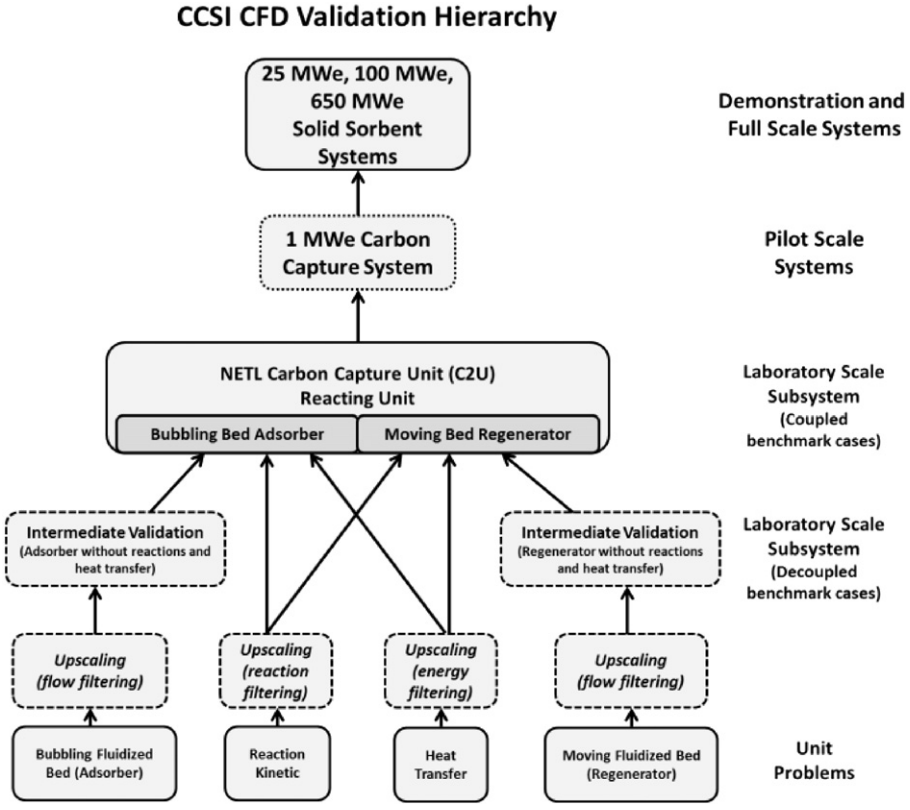

Fig. 1. CCSI hierarchical calibration and validation framework.

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