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Sensitivity study of a full-scale industrial spray-injected fluidized bed reactor

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ABSTRACT

The industrial fluidized bed reactor (FBR) described here is designed to convert an aqueous solid laden stream into a consistent granular product. The FBR is heated to 650 °C and chemically reducing conditions are achieved by using steam as the fluidizing gas and coal as a source of carbon. The objective of this study is to use the MFiX (Multiphase Flow with Interphase eXchanges) two-fluid model as a screening tool to investigate the effects of off-nominal conditions to establish performance guidelines. This information will be helpful in assessing whether the identified boundaries of the system are steep or gradual. Initially, 13 independent operating parameters were sampled in a one-at-a-time manner using high, low, and base values and ranked against a set of performance criteria indicative of defluidization. Five operating parameters were found to have the largest effect (bed particle size, bed particle density, coal particle size, spray feed flow rate, and fluidizing gas flow rate) on three quantities of interest—bed differential temperature, low solids velocity, and bed voidage. Latin-hypercube sampling was used to generate a minimal number of random values for various combinations of input parameters. The spray feed flow rate was the most significant parameter affecting the temperature differences, followed by the coal particle and bed particle size. The bed particle size had the largest effect on the low velocity of the bed particles, with the coal particle size as a contributing second effect. The high solid packing shows the coal particle size with the largest effect, and significant secondary contributions from the feed flow rate and fluidizing gas flow rate. The fits to the five-dimensional Gaussian Process models were 0.7797, 0.8664, and 0.9440 for the temperature, velocity, and solids packing, respectively.

1. Introduction

Fluidized bed reactors (FBRs) are attractive choices for industrial applications involving heterogeneous chemical reactions due to the high heat transfer and reaction rates that occur as a result of the very large specific surface area. The ease of removal and addition of solids to these reactors make them more amenable to continuous processing of feed material than fixed bed reactors. However, there are disadvantages to FBRs, especially when scaling up from bench- to pilot-scale, where circulation patterns can cause regions of poor mixing with consequent issues related to temperature gradients and particle entrainment or metal surface erosion in areas where local gas velocities are high [1]. In addition, the scale-up of fluidized beds is more useful for cold models, and significantly deep beds can cause significant gas bypassing, with poorer gas-solids contact than in pilot plants [2].

A few models exist which are capable of resolving the complex fluid-particle and particle-particle momentum and energy interactions occurring throughout fluidized beds. The review article by Philippsen et al. [3] discusses the important role of hydrodynamic modeling of fluidized beds and surveys the state of the art in modeling and simulation techniques. Papadikis et al. [4] determined that, for predictions of heat, mass and momentum transfer, 3D simulations are more suitable for modeling fluidized beds than simulations performed in 2D. The two-fluid model (TFM) developed by Kuipers et al. [5] considers the gas and solid phases to be continuous and fully penetrating where all relevant terms in the transport equations are retained. The TFM applied to small-scale 2D axisymmetric beds can predict some changes in particle motion and fluid regime transitions, as well as bubble size and velocities in agreement with literature correlations for Geldart Group B particles [6]. With sufficient grid size and time step restrictions, TFM can also predict correct bed expansions [7]. Some large-scale effects, such as pressure drop across the bed in full 3D simulations, can be simulated correctly utilizing the Euler-Euler TFM [8]. Heat transfer characteristics for wall-to-bed heat transfer in the TFM have been shown to be in reasonable agreement with experimental results in both the Symalal-O'Brien [9] and Gidaspow [10] drag models given sufficient simulation time to develop a periodic pattern [11]. A set of coupled heat transfer-reactive flow cases for fast pyrolysis of solid material has shown initial potential utilizing the TFM [12]. More recently, the expanded modeling

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of fast pyrolysis in fluidized beds using the TFM has been shown to match the gas evolution rates with good experimental agreement [13,14]. A TFM, rather than CFD coupled with a discrete element method (DEM), is used to model our full-scale industrial reactor since the number of particles present (~1×10^{10} particles) would far exceed current computational power even given recent advancements in CFD-DEM methods using up to 25 million particles [15]. Thus, for the sensitivity study performed here, DEM would not be feasible and the TFM is used instead.

The MFiX (Multiphase Flow with Interphase eXchanges) general-purpose hydrodynamic code was used to create the FBR model for the sensitivity studies. MFiX simulations provide detailed information on fluid and solids volume fractions, pressure, temperature, gas species, and velocity distributions within the reactor as a function of process parameters. Validation of the granular flow model implemented in the MFiX code for computational fluid dynamics (CFD) modeling of fluidized beds has been performed by Benyahia [16]. Gaussian process modeling has been used for uncertainty quantification within bubbling beds with a good degree of success utilizing the MFiX code [17], although the model here is of a much larger physical and computational size. Similar work has been done with random sampling for Uncertainty Quantification (UQ) in the MFiX code with the module for discrete element particles in fluidized beds to create response surfaces over unknown input parameters [18]. Modeling gasifiers that contain many reactions as a result of the coal injection has been extensively studied using the MFiX TFM as well [19]. Most of the literature data that is available for well-validated systems is on smaller reactors, as obtaining data for large fluidized bed systems can be costly.

The fluidized bed reactor (FBR) system that is studied here primarily revolves around the spray injection of an aqueous reactant into a fluidized bed. The spray is injected by nozzles along one side near the bottom of the FBR, rather than from the top as in typical spray injection systems. The bed is fluidized mainly with steam through a ring header and rail distributor, but also contains a mix of carbon dioxide and nitrogen. Steam is superheated before entering the FBR and adding calcined coal into the bed provides the remainder of the heat needed to achieve the desired operating temperature. A simple representation of the system is shown in Fig. 1.

The chemical conversion process produces a solid, granular product. The overall process uses two fluidized bed reactors, one for converting solid laden aqueous stream into granular bed product and the other for reducing the off-gas and small particulate material. The FBR studied here consists of the first step, where the aqueous feed is solidified by evaporating water and reducing solid compounds. The off-gas from the first FBR system is passed into the second FBR, where the hydrogen, carbon monoxide, and other organics are fully oxidized and cooled prior to venting to the environment.

The FBR is fluidized with steam and heated to an operating temperature of 650 °C using calcined coal and controlled portions of air and oxygen intended to maintain overall stoichiometrically reducing conditions. The reactant is spray-atomized into the fluidized bed of the FBR, where it evaporates and is reacted to decompose initial solid material and convert the dissolved and undissolved solids to the granular solid product. The bed product is periodically removed from the bottom of the FBR and conveyed through a transfer system for storage in containers. The evaporated water and gasified reaction products flow with the fluidizing gas through a set of three parallel cyclones in the upper freeboard, and then through a sintered-metal filter unit for off-gas release and fine particulate removal. Some product fines, attrited bed media, and attrited coal and charcoal particles are entrained in the gas stream and elutriate from the bed. The cyclones capture the larger elutriated particles and return them to the FBR bed via downcomer pipes. The off-gas system captures the remaining elutriated fines, which are transferred to the solids processing unit and eventually combined with the FBR product for transfer into storage canisters. The CFD simulations performed were done to help guide the operation of a fluidized bed reactor which was not performing well prior to reaching its desired pseudo steady state. This resulted in paucity of high quality data for validation of the model lack of data to provide informative Bayesian calibration of the simulation parameters as in Lai et al. [20].

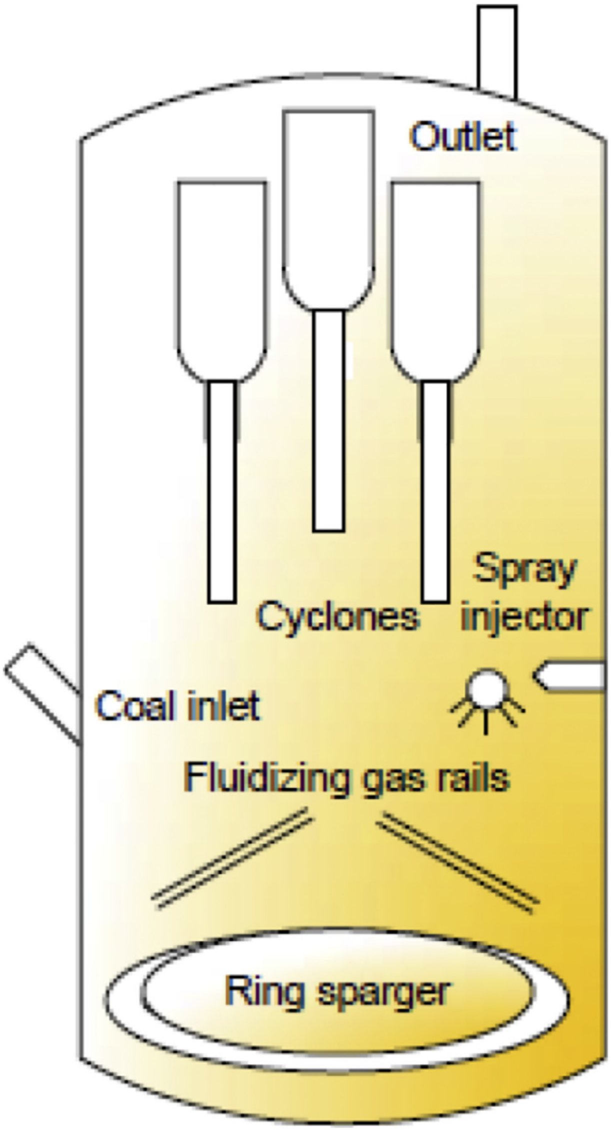

Fig. 1. Representation of the spray-injected FBR.

Operational parameters of the FBR were assessed by performing one-at-a-time sensitivity tests for 13 parameters at high, base, and low values. The base-case operational regime was defined based upon pre-operational tests in the full-scale reactor. The goal of this work is to identify the parameters that have the largest effect on other parameters during operations and the ranges of operational parameters that should be avoided to maintain good fluidization and solids mixing. Three main quantities of interest (QOIs) were identified as: (1) the maximum temperature difference in the central region of the bed, (2) low velocity threshold of solid material, and (3) high-solids packing as indicated by the bed voidage. The results of these one-at-a-time studies were used to narrow down the selection of parameters from 13 to five for additional simulations based on a Latin-hypercube design using the DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) toolkit. Results from the LHS-defined simulations were then analyzed using Gaussian process (GP) models with linear trends to determine the sensitivities [21].