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Large eddy simulations of coal gasification in an entrained flow gasifier

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HIGHLIGHTS

- ▶ Multi-phase turbulent flow and coal gasification in an entrained flow gasifier is simulated using LES and RANS.
- ▶ LES captures unsteady flow structures in both combustion and gasification zones of the gasifier.
- ▶ Unsteady flow structures affect mixing and char-conversion efficiency.
- ▶ LES accurately predicts char-conversion efficiency compared to RANS.

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ABSTRACT

In this paper, we investigate multi-phase reacting flow in a coal-fed entrained flow gasifier using large-eddy simulations and Reynolds-averaged Navier Stokes models, respectively. An axial-flow type lab-scale gasifier is investigated. The simulations are performed using a Lagrangian–Eulerian method in which the coal particles are modeled using a Lagrangian approach and the gas phase is solved using an Eulerian approach. We compare the performance of LES and RANS results. The coal particle models include devolatilization, char consumption that uses heterogeneous chemistry and two-way coupling of mass, momentum and energy with the surrounding gas phase. The gas phase combustion is modeled using homogenous chemistry and the effect of turbulence on combustion and gasification is modeled using a partially stirred reactor approximation. Results show that LES captures the unsteady flow structures inside the gasifier. We show that modeling the unsteady mixing is critical to the accurate predictions of the gas phase species and carbon conversion in these gasifiers.

1. Introduction

Entrained Flow Gasifiers (EFGs) are key component in Integrated Gasification Combined Cycle (IGCC) power plants designed to reduce emissions along with the potential for carbon dioxide capture and the integration with synthetic fuel production. In EFG, gasification converts coal into clean synthetic gas. Entrained flow gasifiers have been designed using zero-dimensional models. There is renewed interest in designing EFGs that can handle different feedstock, and to gain better insight into the gasification process for, e.g., the development of compact and more reliable gasifiers [1]. The flow inside an entrained flow gasifier is inherently unsteady and involves complex turbulent mixing of two phases; coal particles in solid phase and oxygen and steam in the gaseous phase. The gasification process involves phenomena such as devolatilization, heterogeneous surface reactions and complex gas phase chemistry. To develop a fundamental understanding of this multi-phase reactive process, a comprehensive, high fidelity Computational Fluid Dynamics (CFD) model is needed. These higher fidelity models can be used to improve injection strategies for higher carbon conversion efficiency, detect potential failure modes such as the formation of hot-spots that cause thermal wear, and examine the overall reliability and fuel flexibility of different designs.

There are few experimental investigations of entrained flow gasifiers in literature. The available data are mostly limited to lab scale gasifiers and much less for pilot scale gasifiers. Intrusive probe are often used for sampling. Brown et al. [2], performed such experiments in the oxygen fired Brigham-Young University lab-scale gasifier. They obtained temperature and syngas composition measurements along the gasifier axis. This lab-scale gasifier operated at atmospheric pressure and the results covered four different types of coal. Hill and Smoot [3] performed CFD simulations using RANS model on these gasifiers and compared their results with the measured data. In the BYU axial flow gasifier coal particles were injected along with oxygen from a central nozzle and steam was injected from the surrounding secondary nozzle hole as shown in Fig. 1. The Mitsubishi Heavy Industries (MHI) gasifier, on the other

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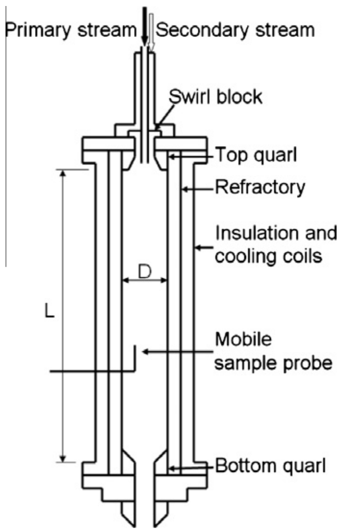

Characteristic	1 tpd BYU lab-scale
Flow direction	Down
Feedstock delivery	Dry
Injector configuration	Axial
Oxidant	O_2
Number of stages	1
Wall lining	Refractory with cooling
Syngas cooling	Quench

Fig. 1. Schematic of BYU gasifier.

hand, is air-blown swirling flow type gasifier. Both research-scale and pilot-scale versions were built, with coal flow rates of 2 tons/day and 200 tons/day, respectively. These gasifiers have two sections, a lower combustion section and an upper gasification section. Coal particles are injected along with air jets tangentially in the combustor section to create swirling flow inside the gasifier. In the gasification section more coal is injected. Various researchers have performed simulations of the MHI two-stage gasifier for both the research scale (Watanabe and Otaka [4]) and the pilot scale (Chen et al. [5,6]).

Two approaches have been used for multiphase reactive flows similar to what is encountered in gasification. These are Lagrangian–Particle Eulerian–Fluid models (LPEF) and Eulerian–Particle Eulerian–Fluid models (EPEF). In the LPEF method, the solid phase particles are tracked using a Lagrangian approach, while the surrounding gas phase is modeled using Eulerian approach. In both cases, the two phases are coupled through source terms in the conservation equations of mass, momentum and energy. In the EPEF method, both the solid and gas phases are solved using an Eulerian approach and an additional equation is solved the "volume fraction", which represents the fractional volume of the solid-phase locally. Typically the EPEF is a good choice for cases in which the solid phase occupies high volume and the velocities of the flow are relatively small [7]. The EPEF method is better for calculating the group effect of the solid phase in regions where the local volume fraction of the solid phase is high. On the other hand, the LPEF method is widely used for flows in which the solid particles are widely dispersed within the flow and the flow velocities are much higher as typically found in EFGs [8]. The LPEF methods have also been used in many other combustion systems, such as diesel engines and gas turbine combustors where liquid droplets are tracked.

Recently there have been several investigations of EFGs using one-dimensional and RANS approach. Monaghan and Ghoniem [9] developed a 1D gasification model using a reactor network. Their model showed good agreement with experimental data along the length of the gasifier. Watanabe and Otaka [4] performed multi-dimensional CFD-RANS simulations using the LPEF method for the research scale MHI gasifier. Kumar and Ghoniem [10] performed computations of entrained flow gasifiers that range from commercial, research and pilot scale gasifiers using different turbulence models in RANS. They found that while k–ε performs well for gasifiers with straight injection, k–ω performs much better for swirling-flow type gasifiers. Gasification processes at the single-particle level have also been modeled at various complexity levels. Kobayahsi et al. [11] and Ubhayaker et al. [12] investigated different coal types to characterize char consumption kinetics and devolatilisation processes. Goetz et al. [13] performed simulations to characterize the impact of char-consumption kinetics. In recent years, Katijani et al. [14] studied char-kinetics and gasification in carbon dioxide and steam in a pressurized drop tube furnace (PTFD). Singer and Ghoniem [15] focused on developing sub-particle structure models and their impact on char consumption. So far, higher fidelity CFD simulations such as LES of coal gasification have not been attempted.

In this paper, we apply LES to simulate coal-gasification processes. LES models can capture some of the unsteady structures that affect mixing, turbulent-chemistry interactions, turbulence dispersion of particles, etc. Data from the Brigham Young University's lab scale gasifier is used to validate the LES simulation. These data include the exit temperature, and gas composition along the length of the gasifier for four different coal types. The measured data also include gas composition distribution in the radial directions of the gasifier at various axial locations. We use the LPEF approach in the open source code OpenFOAM, along with turbulence modeling using the one-equation eddy viscosity model, and compare the results with the k–ε RANS model. Heterogeneous surface reactions, devolatilization, and two-way coupling of particle-gas phase are included.

2. Solid phase numerical model

The solid-phase model accounts for fuel conversion via pyrolysis and char consumption, and particle transport. The particle transport model solves the mass, momentum and energy equations of the particle along the jet trajectories [10]. In the context of coal gasification, we discuss key models used in this investigation, viz., pyrolysis and char conversion chemistry. The BYU gasifier operates at high temperatures near the nozzle region and hence pyrolysis occurs at a very fast rate.

$$\mathrm{Coal} \rightarrow \alpha_1 \mathrm{CH}_x + \alpha_2 \mathrm{H}_2 + \alpha_3 \mathrm{CO} + \alpha_4 \mathrm{CO} + \alpha_5 \mathrm{H_2O} + \alpha_6 \mathrm{N}_2 + \alpha_7\ \mathrm{Char} \tag{1a}$$

$$\sum_i \alpha_i = 1 \tag{1b}$$

Consistent with Badzioch's and Hawksley's [16] approach, the devolatilization rate is given by a single kinetic rate that is similar to the Arrhenius form.

$$\frac{dm_V}{dt} = -A \exp\left(-\frac{E_0}{\mathrm{RT}}\right) m_V \tag{2}$$

where m_V is the mass of the volatiles remaining in the particle, $A = 2.1\times10^6\ \mathrm{s}^{-1}$ and $E_0 = 2.1\times10^7$ J/kmol, and T is the temperature of the particle. The devolatilization process is assumed to energetically neutral since the heat of devolatilization is negligible as compared to heat of reactions due to char consumption and combustion reactions.

2.1. Char conversion chemistry

The coal particle is left with char and ash after all the volatile components are released. Char reacts in the presence of steam, oxygen and carbon dioxide and gets converted into carbon monoxide and hydrogen.

$$\mathrm{C} + 1/2\mathrm{O}_2 \rightarrow \mathrm{CO} \tag{3a}$$

$$\mathrm{C} + \mathrm{CO}_2 \rightarrow 2\mathrm{CO} \tag{3b}$$

$$\mathrm{C} + \mathrm{H_2O} \rightarrow \mathrm{CO} + \mathrm{H}_2 \tag{3c}$$