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Application of a validated gasification model to determine the impact of coal particle grinding size on carbon conversion

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HIGHLIGHTS

- ▶ The C–O_2 reaction is diffusion-limited, while the C–CO_2/C–H_2O reactions are kinetics-limited under the tested conditions.
- ▶ Grinding finer than ~134 μm speeds up carbon conversion in the GE gasifier and combustor section of the MHI gasifier.
- ▶ Fine grinding does not accelerate carbon conversion at the diffuser section of the MHI gasifier.
- ▶ Particles smaller than 36 μm undergo complete conversion within the oxygen-rich sections in both the MHI and GE gasifiers.
- ▶ The larger particles primarily convert through the C–CO_2 and C–H_2O reactions in the latter stages of the gasifiers.

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ABSTRACT

In this paper, we describe the implementation of a comprehensive, previously validated multiscale model of entrained flow gasification to examine the impact of particle size on the gasification process in two different gasifier designs; the MHI and the GE gasifier. We show that the impact of the particle size depends on whether the char conversion process is kinetically limited or boundary layer diffusion-limited. Fine grinding helps accelerate char conversion under diffusion-control conditions, whereas the impact is not as noticeable under kinetic-control operation. The availability of particular gasification agents, namely O_2 in the earlier sections of the gasifier or CO_2 and H_2O in the latter sections, as well as the temperature, are shown to have an impact on the relative importance of kinetics versus diffusion limitation.

1. Background and motivation

The design of coal gasifiers has been largely an experience-based enterprise. Many of the present gasifiers are susceptible to several failure modes including refractory damage, injector blockage or burn-out and slag port blockage. Moreover, it is unclear whether the accepted operational practices are optimal with respect to parameters such as the reactor pressure, mass throughput, injection swirl, angle of injection in case of tangential injection, dimensions of critical regions, extent of feedstock grinding. A comprehensive, validated CFD model is instrumental in ascertaining whether important gasifier performance metrics like carbon conversion and cold gas efficiency are optimized with respect to the relevant parameters.

A multiscale model of entrained flow gasification has been developed and validated at the level of individual critical submodels including the turbulence model and the particle turbulent dispersion model in [1]. In addition, the overall model has been validated for a variety of gasifiers operating under different conditions including air-blown to oxygen-blown, atmospheric pressure to pressurized, pilot-scale to lab-scale, tangentially-injected to axially injected conditions in [2]. In this work, the validated model is applied to examine the impact of changing the particle size on the performance of two widely used units: the MHI and the GE gasifiers.

Determining the impact of the particle size on carbon conversion is critical for two reasons:

(1) Depending on the particular gasifier design and the stoichiometric ratio within specific regions of the gasifier, as discussed in the next section, fine grinding of coal may or may not have a significant impact on

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Nomenclature

Capital letters
A_p particle external surface area (m^2)
C fractional particle conversion rate (1/s)
P_i partial pressure of species i (Pa)
S char particle internal surface area (m^2/kg)
T_g gas phase temperature (K)
T_p particle temperature (K)

Lowercase Letters
d_p particle diameter (m)
k_d diffusion reaction rate constant (kg/atm s)
k_s kinetics reaction rate constant (kg/atm s)
m_p mass of a tracked Lagrangian particle (kg)
$t_{conversion}$ time taken for carbon conversion
x fractional carbon conversion

Arrhenius constants
k_{11} $0.45\exp(-212/RT)$ g/atm s cm^2
k_{12} $0.021\exp(23/RT)$ 1/atm
k_{13} $0.038\exp(48.1/RT)$ 1/atm
k_{21} $32.8\exp{-209.2/RT)}$ g/atm s cm^2
k_{22} $4.9e-5\exp(-24.5/RT)$ 1/atm
k_{23} $1.1e-7\exp(114.1/RT)$ 1/atm$^{0.5}$
k_{31} $30\exp(-30/RT)$ atm$^{0.35}$/s

carbon conversion rate. Accurate modeling can reveal this dependence and help make informed decisions.

(2) Studies have indicated that there is a premium on fine grinding of coal. Although the grinding energy itself might remain as a small fraction of the heating value, which depends on the coal, a more stringent requirement on grinding leads to a reduction in the mill capacity. The extent of reduction depends on the particular grinding mill employed and the grindability index of the coal used [3].

2. Char consumption model

In order to explain the results regarding the impact of the particle size on char conversion, we need to invoke certain aspects of the char consumption model, especially the description of the char consumption rate under complete kinetic control and complete boundary layer diffusion control. The model is described in detail elsewhere [2].

The char consumption rate via C–CO_2 reaction, in the regime where kinetic control can be assumed, is written as [4]:

$$\begin{aligned}\dot{m}_p &= k_s p_g \\ &= m_{p0} s_0 (1-x)\sqrt{1-\psi\ln(1-x)}\frac{k_{11}p_{co_2}}{1+k_{12}p_{co_2}+k_{13}p_{co}}\end{aligned} \tag{1a}$$

where m_{p0} is the initial char mass of the particle, S_0 is initial internal surface area (m^2/kg), x is the instantaneous particle char conversion, ψ is the structural parameter for the random pore model taken as 1.0 for the present coal, k_{1i}'s are the Arrhenius constants, and P_{CO_2} and P_{CO} are the free stream partial pressures of CO_2 and CO, respectively, in the vicinity of the particle. This rate expression is 'intrinsic', since it depends on S_0. Similar expression for the C–H_2O reaction, in the kinetics-controlled regime, is written as [5]:

$$\begin{aligned}\dot{m} &= k_s P_g \\ &= m_{p0} S_0 (1-x)\sqrt{1-\Psi\ln(1-x)}\frac{k_{21}P_{H_2O}}{1+k_{22}P_{H_2O}+k_{23}\sqrt{P_{H_2}}}\end{aligned} \tag{1b}$$

where k_{2i}'s are the Arrhenius constants, and P_{H_2O} and P_{H_2} are the free stream partial pressures of H_2O and H_2, respectively, in the vicinity of the particle. An nth order extrinsic rate expression is used for the C–O_2 reaction [6]:

$$\dot{m}_p = k_s P_g^n = m_{po}(1-x)\sqrt{1-\Psi\ln(1-x)}k_{31}P_{O_2}^n \tag{2}$$

where k_{31} is the Arrhenius constant, n is −0.35 and P_{O_2} is the free stream partial pressure of O_2 in the vicinity of the particle. The values of all the Arrhenius constants are provided in the nomenclature section of this article. As shown later in this paper, the C–O_2 reaction is typically limited by diffusion through the boundary layer. Under complete diffusion control, the char consumption rate is given as:

$$\dot{m}_p = P_g k_d = A_0 P_g \frac{A_d}{P d_p}\left(\frac{T_g}{2000}\right)^{0.75} \tag{3}$$

where A_0 is the external surface area of the particle (m^2), A_d is a constant and depends on the corresponding gas-phase reactant, P_g is the free stream partial pressure of the gas-phase reactant, T_g is the gas-phase temperature in the vicinity of the particle, P is the total pressure and d_p is the particle diameter. Relations (1)-(3) will be employed in the following sections to develop scaling relations for the dependence of particle conversion rate on the relevant physical quantities such as reactor pressure and particle diameter.

3. Results for MHI pilot-scale gasifier

The application and validation of the CFD model with respect to the pilot-scale and research-scale MHI gasifiers is described elsewhere [2]. In this section, we utilize the 200 tons/day pilot-scale MHI gasifier model to perform a sensitivity analysis with respect to the particle size. The MHI gasifier, depicted in Fig. 1, incorporates three different dry-feed injectors. The first two are within the combustor region, where oxygen is available for reaction with the volatiles and the char. The third injector is in the diffuser. Our numerical analysis and the experimental data reported in [7] indicate that this gasifier typically produces lower carbon conversions, 70–90%, and char recycling is required. Recycled char is injected through the combustor char burner (injector 2 in Fig. 1). Approximately 55% of the total coal is injected at the diffuser burner and the rest at the combustor burners, whereas only 15% of the total air is injected at the diffuser burner with the remaining 85% being injected at the two combustor burners.

Taiheiyo sub-bituminous coal (TH) [6,7] is modeled in our work. The coal properties and the gasifier operating parameters used in this work are listed in Tables 1 and 2, respectively.

Fig. 2a shows the variation of the oxygen mole fraction within the gasifier. Oxygen is available within the lower combustor section and only close to the injectors near the char combustor burner. Oxygen concentration is negligible in the diffuser burner, especially compared to the amount of coal injected at that location. The combustor stage primarily produces CO_2 and H_2O, and thermal energy through the combustion of volatiles, recycled char and some of the coal with O_2, which are then used to gasify the coal injected within the diffuser and reductor regions to yield CO and H_2 as the final products.