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Entrained flow gasification. Part 2: Mathematical modeling of the gasifier using RANS method



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ABSTRACT

CFD (RANS based) simulations of REGA-1 experimental campaign concerning gasification of glycol in an oxygen-nitrogen mixture have been carried out. The reacting flow-field has been computed using a number of turbulence models while turbulence-chemistry interactions have been modeled using either the Eddy Dissipation Concept (EDC) or the presumed PDF approach. Two global-chemistry schemes have been used: the (HVI1) scheme for glycol gasification and the extended Jones-Lindstedt scheme. Radiation has been computed using the Discrete Ordinate Method with a comprehensive analysis concerning absorption/emission of infrared radiation by gaseous molecules as well as absorption and scattering on droplets. The CFD-predictions of the near-atomizer region have been sensitive to and strongly dependent on the sub-models used; the spray sub-model and the chemical schemes are the most important. Good quality predictions of temperature and chemical species (CO, H₂, CO₂, H₂O, CH₄) concentrations at 300 mm and 680 mm distances from the atomizer have been obtained. The HVI1 global chemistry scheme has predicted very well not only the CO/CO₂ ratios but also the trace concentrations of methane. The paper shows how to simplify the radiative heat transfer simulations without a significant loss in accuracy.

1. Introduction and objectives

The modeling and simulation of entrained flow gasification has been a challenge for more than four decades. Due to various designs of entrained flow gasifiers (two-stage up-flow, one-stage down-flow) and different operating conditions (in particular pressure), a great number of studies have been performed. The studies, up to the 1990s, used mainly one-dimensional models of coal gasification (see e.g. Wen [1], Govind [2]) but, despite large dimensions of entrained flow gasifiers, and limited computer resources of the time, few CFD studies [3–11] have also been performed. Since then the number of works based on CFD calculations has significantly increased. Although most of these studies considered different kinds of gasifiers and used different CFD codes (in-house, Fluent, ANSYS Fluent, CFX, OpenFOAM), there are quite a few similarities, namely the use of a RANS turbulence model or the employment of a simplified reaction mechanism for the gas-phase kinetics based on the publications of Westbrook and Dryer [12], and Jones and Lindstedt [13]. Reactions of the char with CO₂, H₂, H₂O and O₂ have often been implemented employing kinetics either taken from literature or measured. Radiation has been described using one of the

common models (Discrete Ordinate Method (DOM), P1 model, Discrete Transfer Radiation Model (DTRM)). Many research groups have carried out simulations to improve sub-models (e.g. devolatilization, chemical reactions, and slagging), to generate information important for the gasifier design, or to demonstrate that a CFD model can be applied to compute both the composition and the temperature at the gasifier exit. Sensitivity analysis of operating parameters (O₂/C-coal ratio, H₂O/C-coal ratio, coal type, coal properties) and unknown model parameters (e.g. homogeneous and heterogeneous reaction rates) have often been carried out [8–11].

Brown et al. [3,4] investigated coal gasification and measured concentrations of CO, CO₂, H₂, and H₂O at different axial and radial positions in the Brigham Young University (BYU) atmospheric entrained flow gasifier. They employed the PCGC-2 CFD code to compare the simulation results with the measured data and to analyze the effects of gas-phase chemistry, heterogeneous reaction rates, and operating conditions.

Fletcher et al. [6,7] carried out simulations of biomass gasification in an up-flow gasifier and investigated sensitivity of the predictions to the turbulence model used. They concluded that inside the diffuser

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Nomenclature*Greek letters*

β	second viscosity (kg m/s)
δ_{ij}	Kronecker delta
ϵ_p	droplet emissivity
η	wavenumber (m)
γ^*	fine structure mass to the total mass ratio
μ	dynamic viscosity (Pa s)
ν_p	stoichiometric coefficients for products
ν_r	stoichiometric coefficients for reactants
Ω	solid angle (str)
Φ	dissipation by viscous stress (kJ/(m ³ s))
Φ_η	scattering phase function
ρ	density (kg/m ³)
ρ_p	droplet density (kg/m ³)
σ	Stephan-Boltzmann constant (W/(m ² K ⁴))
σ_f	variance of the mixture fraction
$\sigma_{\eta,s}$	gas scattering coefficient (1/m)
τ^*	Eddy characteristic time scale (s)
τ_e	Eddy characteristic lifetime (s)
θ_R	radiation temperature (K)
ϵ	turbulent energy dissipation (m ² /s ³)
ξ	limiting factor for reaction rate in the fine structures

Non-dimensional numbers

B	Spalding mass transfer number
Nu	Nusselt number
Pr	Prandtl number
Re	Reynolds number
Re_p	droplet Reynolds number
Sc	Schmidt number
Sh	Scherwood number

Roman letters

\dot{m}_e	evaporation rate per unit of surface (kg/(m ² s))
	MEG mass flow rate (kg/h)
\dot{m}_{N_2}	nitrogen mass flow rate (kg/h)
\dot{m}_{O_2}	oxygen mass flow rate (kg/h)
\dot{Q}	heat source/sink (kJ/(m ³ s))
\dot{q}_w	wall heat flux (kW/(m ² s))
\dot{s}_m	mass sources (kg/(m ³ s))
\mathbf{a}_d	acceleration due to drag force (m ² /s)
\mathbf{D}	stress tensor (kg/(m ² s))
\mathbf{g}	gravity acceleration (m ² /s)
\mathbf{J}	mass transfer flux (kg/(m ² s))
\mathbf{J}_t	turbulent mass transfer flux (kg/(m ² s))

\mathbf{q}_c	heat flux vector (kW/m ²)
\mathbf{q}_m	multicomponent enthalpy flux vector (kW/m ²)
\mathbf{q}_t	turbulent enthalpy flux vector (kW/m ²)
\mathbf{T}	turbulent Reynolds Stress tensor (kg/(m ² s))
\mathbf{u}_{rel}	relative velocity (m/s)
\mathbf{U}	fevre averaged gas velocity (m/s)
\mathbf{u}_p	droplet velocity (m/s)
\mathbf{x}_p	droplet position (m)
A	Arrhenius rate constant
A_p	droplet external surface (m ²)
a_η	spectral gas absorption coefficient (1/m)
a_f	forwards reaction order
a_k	absorption coefficient for band k (1/m)
a_r	backwards reaction order
b	temperature exponent
c_p	droplet specific heat capacity (kJ/(kg K))
d_p	droplet diameter (m)
D_t	turbulent molecular diffusivity (kg/(m s))
D_{eff}	effective molecular diffusivity (kg/(m s))
$D_{i,m}$	molecular diffusivity (m ² /s)
E	activation energy (J/kmol)
e	specific total energy (kJ/kg)
f	mixture fraction
h	specific enthalpy (kJ/kg)
h_g	convective coefficient (kW/(m ² K))
I_k	radiation intensity in band k (W/str)
$I_{\eta,b}$	black body spectral intensity (W/(str m))
I_η	spectral intensity (W/(str m))
$I_{k,b}$	black body intensity for band k (W/str)
k	turbulent kinetic energy (m ² /s ²)
k_e	mass transfer coefficient (kg/(m ² s))
k_g	gas thermal conductivity (kW/(m K))
k_t	turbulent thermal conductivity (kW/(m K))
k_w	wall thermal conductivity (kW/(m K))
k_b	backwards reaction rates constant
k_{eff}	effective thermal conductivity (kW/(m K))
k_f	forwards reaction rates constant
m_p	droplet mass (kg)
p	pressure (Pa)
R	universal gas constant (J/(kmol K))
r_{ev}	specific evaporation enthalpy (kJ/kg)
T	gas temperature (K)
T_∞	local temperature of the gas-phase (K)
T_{he}	temperature of the heating elements (K)
T_p	droplet temperature (K)
T_w	wall temperature (K)
u'_i	turbulent velocity fluctuation (m/s)
w_k	temperature weighting function for band k
Y	mass fraction

section, the flow could be better predicted by applying the Differential Reynolds Stress Model than the standard $k-\epsilon$ model. The simulations provided results consistent with measurements.

Chen et al. [8–11] and Liu et al. [14–17] performed extensive sensitivity, design and scale-up studies for two-stage coal gasifiers applying a computer code based on the standard $k-\epsilon$ model and the Multi Solid Progress Variable approach. Vicente et al. [18] employed the Eulerian-Eulerian concept in contrast to many other research groups which used the Eulerian-Lagrangian approach. It was shown that the Eulerian-Eulerian concept is suitable to predict the gasification even though the measured values could only be poorly predicted.

For the DP-1 Pressurised Entrained-flow High Temperature Black Liquor Gasifier, Marklund et al. [19,20] used the CFX code and

performed sensitivity studies of the effect of black liquor physico-chemical properties (specific heat) and the gas-phase absorption coefficient on the model performance. It was pointed out that the physico-chemical properties did not exert a significant influence on the predictions and that the devolatilization of black liquor (including the release of sulfur) had to be described accurately. Comparison of the predicted and measured temperatures inside the reactor indicated substantial differences. This was attributed to both, simplicity of some sub-models and usage of guessed values for parameters to which the predictions were sensitive. In the work of Carlson et al. [21] comparisons of the predictions with gas compositions measured at one point inside the gasifier near the outlet indicated a good agreement. To improve the agreement with measurements one third of the formed

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