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Reaction-diffusion model for steam gasification of single char particle: Implementation using finite difference method

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Numerical simulations are powerful tools to study and analyze gasification processes. Among the applicable models, Computational Fluid Dynamics (CFD) models allow a detailed description of the phenomena taking place inside gasification reactors [1, 2]. The aim of this work is to provide a tool for the development of the terms associated to reaction kinetics needed for CFD models. Thus, the unsteady state steam gasification of a spherical porous char particle using the reaction-diffusion model, presented by [3], is implemented. This model simultaneously describes the kinetics of gasification reactions and the diffusion transport of gaseous species inside the particle.

A spherical porous particle of char of radius $r_p = 4.8$ mm surrounded by steam at constant temperature and pressure is considered. The particle is consumed, maintaining its radius, as the steam and the gaseous species formed by the reactions are transported through the pores of the particle, according to the gasification reactions given by [3], which are: $\mathrm{C} + \mathrm{H_2O} \rightarrow \mathrm{CO} + \mathrm{H_2}$, $\mathrm{C} + 2\,\mathrm{H_2} \rightarrow \mathrm{CH_4}$, $\mathrm{C} + \mathrm{CO_2} \rightarrow 2\,\mathrm{CO}$, $\mathrm{CH_4} + \mathrm{H_2O} \rightarrow \mathrm{CO} + 3\,\mathrm{H_2}$, $\mathrm{CO} + \mathrm{H_2O} \rightleftarrows \mathrm{CO_2} + \mathrm{H_2}$.

The transport equation for each species inside the particle in spherical coordinate system, considering homogeneous behavior in both azimuthal and polar angles, is:

$$\frac{\partial C_i}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\, D_i\, \frac{\partial C_i}{\partial r}\right) + R_i \qquad (i = \mathrm{H_2O},\, \mathrm{H_2},\, \mathrm{CO},\, \mathrm{CO_2},\, \mathrm{CH_4},\, \mathrm{C}) \tag{1}$$

where C_i, D_i and R_i are the concentration, the effective mass diffusivity and the net rate of generation of the given species, respectively, r is the distance in the radial direction and t represents the time. Here, the effective mass diffusivity of each species depends on the porosity of the char particle, which depends on the concentration of C, according to the following equations:

$$\frac{D_i}{D_{i,0}} = \left(\frac{\varepsilon}{\varepsilon_0}\right)^2 \qquad \varepsilon = \varepsilon_0 + \left(1 - \frac{C_{\mathrm{C}}}{C_{\mathrm{C},0}}\right)(1 - \varepsilon_0) \tag{2}$$

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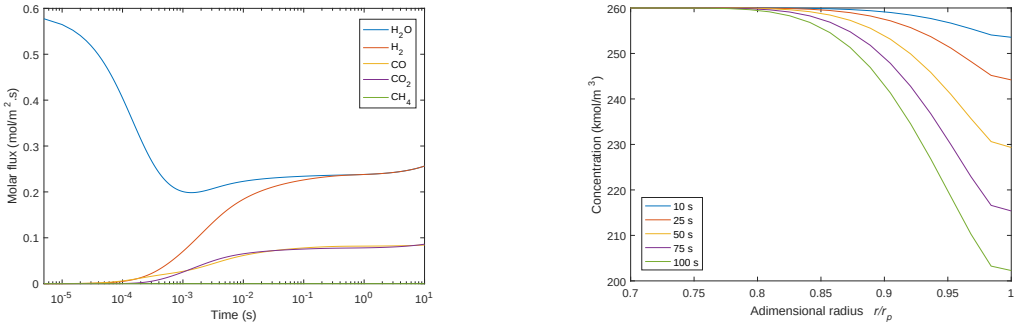
where $D_{H_2O,0} = 2.00 \times 10^{-5}$, $D_{H_2,0} = 1.41 \times 10^{-5}$, $D_{CO,0} = 2.15 \times 10^{-5}$, $D_{CO_2,0} = 1.67 \times 10^{-5}$, $D_{CH_4,0} = 2.93 \times 10^{-11}$ and $D_{C,0} = 0$ are the initial effective mass diffusivities in m^2/s, $\varepsilon_0 = 0.2$ is the initial porosity of the char particle, ε is the porosity at time t, $C_{C,0}$ is the initial concentration of C and C_C is its concentration at the given time. The expressions for R_i can be found in [3]. In addition, the initial concentration of C is $C_{C,0} = 2.6 \times 10^5$ mol/m^3 without any gaseous species inside the particle. Symmetry condition at the center of the particle and constant steam concentration $C_{H_2O} = 1.5$ mol/m^3 together with zero concentration of other gaseous species on its surface are considered.

The model equations are solved using the finite difference method for the spatial discretization coupled to a time stepping method available in built-in functions of MATLAB®. Figure 1(a) shows the molar fluxes of gaseous species crossing the particle surface on a logarithmic time scale for T = 1300 K. It can be observed that after a short initial transient period, the molar fluxes reach to some stationary values. However, a longer simulation time is required in order to characterize the behavior of the process. Figure 1(b) shows the concentration profiles of C for different times at the same temperature.



(a) (b)

Figure 1: Simulation results for T = 1300 K: (a) Molar fluxes of gaseous species crossing the surface, (b) concentration profiles of char at different times.

This is an initial work dedicated to develop CFD models to simulate gasification processes. Further simulation and analysis will be performed.

References

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