

MODELING OF A HIGH-TEMPERATURE DIRECT COAL GASIFICATION PROCESS IN A TWO-STREAM REACTOR

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ABSTRACT

A new scheme for direct gasification of pulverized coal has been analyzed by a mathematical model. Gasification occurs in the annular region of a cylindrical reactor during the cocurrent flow of a steam/coal mixture, with combustion products in the reactor core region serving as an internal heat source. The model incorporates the two equation model for turbulence, mass exchange between phases due to chemical reactions and radiative heat transfer. Detailed calculations are carried out to assess the feasibility of the scheme.

INTRODUCTION

The basic concept for a two-stream gasifier for pulverized coal has been described in earlier publications (see reference 1). The basic configuration is shown in figure 1. Steam and coal are introduced on the periphery of the reactor while air and coal are injected as the core flow. It is assumed that the gasification will occur in the annular region of the cylindrical reactor during the cocurrent flow of a coal/steam mixture with hot combustion products in the reactor core region, the latter serving as the heat source. In this manner, the scheme capitalizes on two well known gasification concepts: direct supply of heat from internal combustion and hydrodynamic separation of gasification products from the combustion gases. The product gases, acceptably clean, are ducted away at the end of the reactor through an annular slot while the combustion gases from the core region are utilized for heat recovery in the system.

A global analysis of the system shows that the scheme is feasible provided that:

- a) sufficient radiative heat transfer occurs between the two streams in cocurrent flow to ensure the completion of the gasification process and,
- b) proper fluid dynamic conditions are achieved to avoid intensive mixing of the two streams in the reactor.

An experimental investigation of the process and the conditions which satisfy these requirements would require costly and extensive experimentation. We have chosen to develop a computer model as the first phase of a research program aimed at establishing the potential feasibility of the scheme and elucidating the important parameters in system design. If the scheme appears feasible, the results of the numerical model will be used to complement design of the experimental rig.

MATHEMATICAL MODEL

The mathematical model of the gasification process entails solving the appropriate conservation equations for the gas and particle phases, as well as a number of auxiliary equations which describe various phenomena and interactions in the process. The model is based on the following assumptions:

- the process is adiabatic.
- the flow and temperature fields are axisymmetric.
- chemical reactions are first order reactions.
- thermal radiation is monochromatic and scattering due to the particles is isotropic.

The gas phase is described by a system of time-averaged conservation equations for momentum, mixture enthalpy and concentrations of chemical species. In addition the equation set contains conservation equations for the kinetic energy and dissipation rate of turbulence following the well known $k - \epsilon$ model (2). The general form for the conservation equations is

$$\frac{\partial}{\partial x}(\rho U \phi) + \frac{1}{r} \frac{\partial}{\partial r}(\tau \rho V \phi) = \frac{\partial}{\partial x}(\Gamma_{\phi} \frac{\partial \phi}{\partial x}) + \frac{1}{r} \frac{\partial}{\partial r}(\tau \Gamma_{\phi} \frac{\partial \phi}{\partial r}) + S \quad (1)$$

where U and V are the axial and radial velocity components and the dependent variable ϕ represents the density, velocity components, turbulence parameters, enthalpy and concentration of chemical species. The chemical composition of the gases is assumed to be nitrogen, oxygen, carbon dioxide, water vapor and gasification products (carbon monoxide and hydrogen). The transfer function Γ_{ϕ} represents such quantities as effective viscosity, thermal conductivity and diffusion coefficients. The source term S incorporates such phenomena as production or depletion of chemical species due to chemical reaction and the mass, momentum and energy sources provided by the particle phase. The definition of these terms will not be included in the interest of brevity.

In order to evaluate thermal radiation exchange, the number density of the particles is needed. Equation 1 is utilized with the transfer function being the effective diffusion coefficient, as taken from Melville and Bray (3), and the source term being zero. The influence of the particulate phase on the effective viscosity of the gas is also modeled with a corrective factor based on the local mass concentration of the particles.

The thermal radiation is simulated with the "six-flux" model (4) with the assumption that the gas radiation is a volume phenomena and the particle radiation is a surface phenomena. It is also assumed that the radiation scattering by the particles is isotropic. Two diffusion-type equations are solved for the radiative heat flux in the axial and radial directions.

The particle velocities and temperatures are obtained by integrating the momentum and energy equations along trajectories for single particles. The effect of particle dispersion due to turbulence is accounted for by adding a "diffusive" velocity to the particle motion which is proportional to the concentration gradient and the effective diffusion coefficient (5). The particle energy equation relates the change in thermal energy of the particle to the convective and radiative heat transfer as well as the energy associated with the change of phase.

To simplify the gasification model, the coal is regarded as char. The mass rate of change of the coal particle is given by

$$\frac{dm_p}{dt} = \dot{r}_c + \dot{r}_g \quad (2)$$

where \dot{r}_c is the reaction rate for combustion and \dot{r}_g for gasification. It is assumed that chemical kinetic and diffusion processes occur in parallel so the reaction rates are given by

$$\dot{r}_g = m_p A_p \rho X_{H_2O} / \left[m_{H_2O} \left(\frac{1}{K_g} + \frac{d_p}{ShD} \right) \right] \quad (3a)$$

$$\dot{r}_c = 1.5 m_p A_p \rho X_{O_2} / \left[m_{O_2} \left(\frac{1}{K_c} + \frac{d_p}{ShD} \right) \right] \quad (3b)$$

where ρ is the gas density, A_p is the particle cross-sectional area, X_{O_2} and X_{H_2O} are the mass fractions of oxygen and water vapor, m is the molecular weight, Sh is the Sherwood number and d_p is the particle diameter. The chemical reaction rates are given in the form of Arrhenius expressions with coefficients determined experimentally for Yugoslav coals (6); namely,

$$K_g = 1.2 \times 10^6 \exp\left(-\frac{23077}{T}\right) \quad (4a)$$

$$K_c = 5.6 \times 10^4 \exp\left(-\frac{15035}{T}\right) \quad (4b)$$

It must be mentioned that these coefficients can vary by an order of magnitude or more depending on the literature source.

The phase coupling in the model is accomplished using the PSI cell scheme (7). Particles are released from a discrete number of radial locations to simulate an initially uniform particle number density. The number flow rate along each trajectory is constant. The change in particle mass, momentum and energy are recorded as each trajectory traverses a computational cell and these become the source terms in the gas-phase flow equations. The energy source term also includes the radiative heat transfer from the particles.

The boundary conditions for the gas phase follow the standard formulations used in conjunction with the $k - \epsilon$ turbulence model (2). The gradient for the concentration of the chemical species is set equal to zero at the wall. Also the incident radiation at the wall is set equal to the wall radiation.

MODEL PREDICTIONS

The verification of the computational model has been partially achieved through its application to simple flow fields for which data are available. Reasonably good agreement between model predictions and experimental results has been achieved for turbulent flows in a circular pipe (8) and a "cold" model of the gasification reactor (9). Verification of the model under realistic conditions for the reactor has yet to be established.

The model was applied to reactor geometry for which the lip separating the two streams was set at a radius ratio of 0.8. The initial velocity of the inner core flow was 6.4 m/s while a velocity of 3.87 m/s was selected for the annular flow. The initial temperature of the inner flow was 1300 K and that of the outer flow was 900 K.

The development of the axial velocity profile at progressive distances downstream is shown in figure 2. There is a rapid mixing initially and momentum diffuses into the low speed outer annular flow to increase the velocity. The temperature of the core stream increases rapidly with the combustion of the coal and there is a consequent acceleration of the flow to satisfy mass flow continuity because of the decreased gas density. Then radiative heat transfer to the outer stream cools down the core flow and heats the outer flow giving rise to velocity changes in each stream (decelerating the core flow and accelerating the annular flow) which drive them both toward velocity equilibrium.

The radial profiles for the gasification products, H_2 and CO , at progressive downstream locations are shown in figure 3. One notes that the gasification products remain basically in the outer region of the reactor and could be separated by an annular slot shown schematically in figure 1. This prediction supports the feasibility of the concept.

The fraction of coal consumed in the gasification process is shown in figure 4. One notes that 60% of the coal at the outside of the reactor has been gasified at approximately five reactor radii from the inlet. Of course, the rate of coal consumption will depend strongly on the gasification rate for specific coals.

The predicted isotherms are shown in figure 5. One notes a very rapid temperature change at the reactor inlet due to combustion of the coal and the subsequent decrease in temperature as the heat is radiated from the hot core to the annular flow. The gas composition at three duct diameters downstream from the inlet is shown in figure 6. One notes, as also shown in figure 3, that the gasification products remain in the peripheral region while the combustion products are concentrated in the core. As shown in the figure, if the slot for the removal of the gasification products were located at a radius ratio of 0.7, the recovery would be primarily CO and H_2 with some CO_2 and water vapor. The relative fractions of chemical species in the slot would be

$$CO + H_2 = 0.54$$

$$CO_2 = 0.16$$

$$H_2O = 0.05$$

$$N_2 = 0.25$$

Of course, the fraction of gasification products to combustion products can be increased by increasing the radius ratio of the slot. However the yield of the gasification products would be reduced. The optimum design remains to be established.

CONCLUSION

Based on the predictions of the mathematical model, the proposed gasification concept appears feasible. The scheme is attractive because of the direct contact heat exchange and the separation of combustion and gasification products. The ultimate assessment of the scheme will only be possible through well-designed pilot plant tests in which the operational conditions and configurations are changed to achieve an optimum design. The numerical model developed here will be a useful tool to complement the design and operational adjustments of an actual system.

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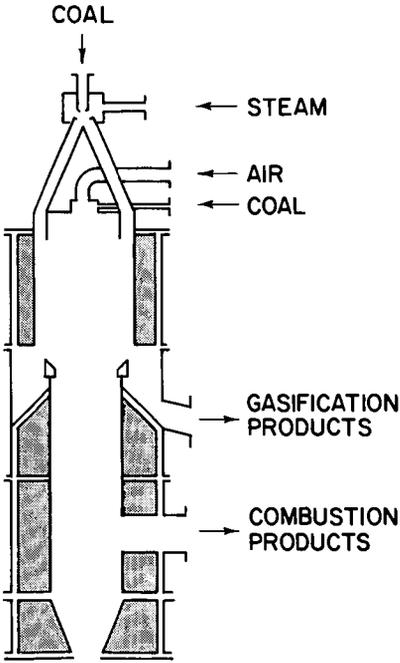


Figure 1. Schematic Diagram of Gasification Reactor.

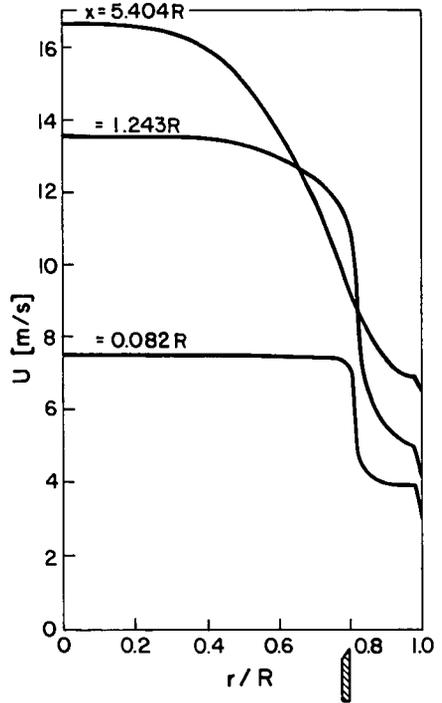


Figure 2. Development of axial velocity profile along reactor.

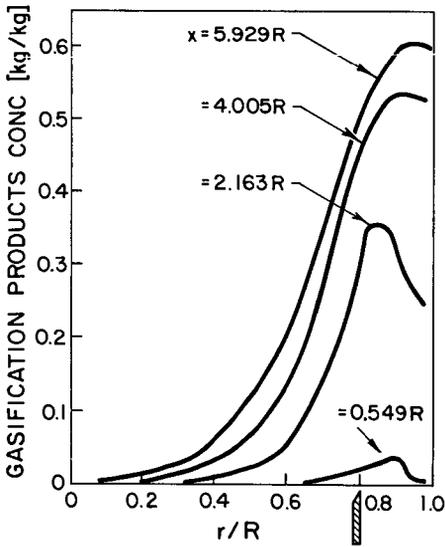


Figure 3. Development of concentration profiles for gasification products along reactor.

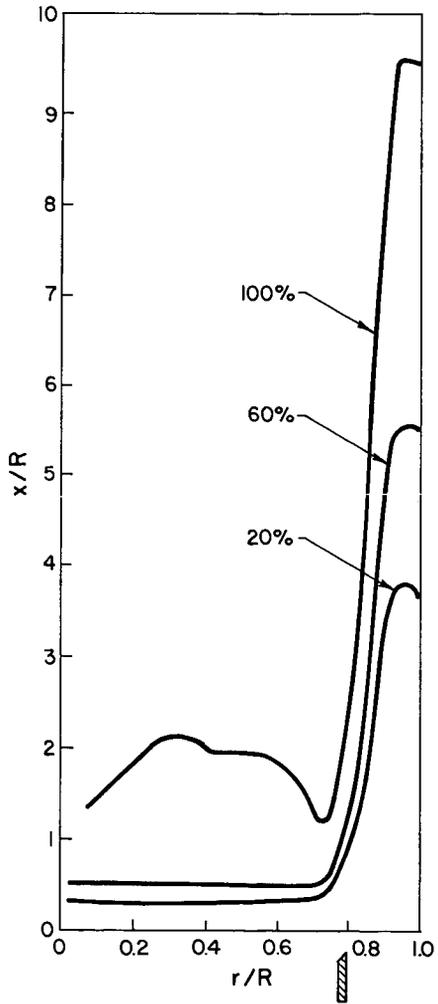


Figure 4. Fraction of coal particle consumption along reactor.

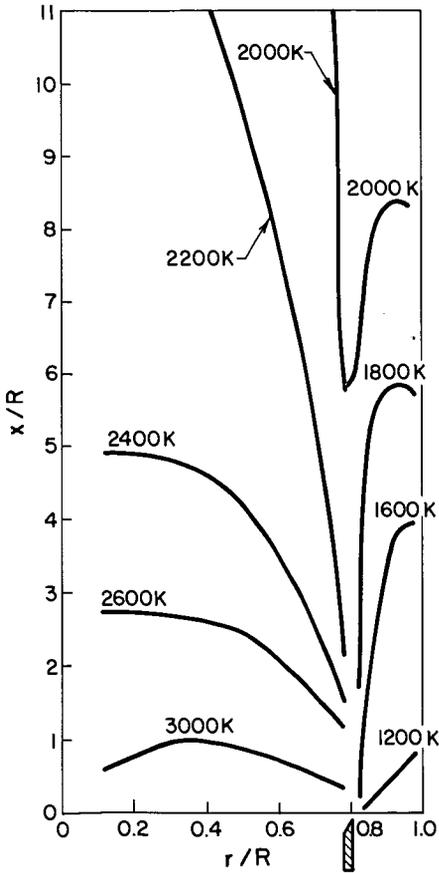


Figure 5. Isothermal profiles in reactor.

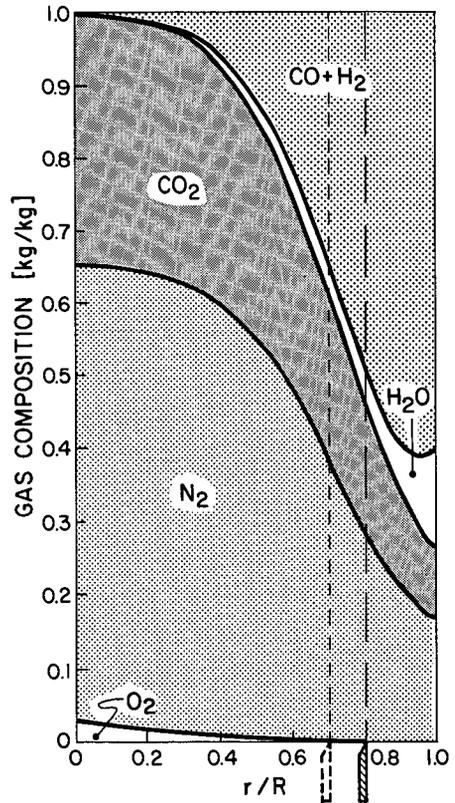


Figure 6. Radial gas phase composition at three duct diameters from inlet.