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THEORETICAL MODELS FOR RATES OF HETEROGENEOUS REACTIONS DURING COMBUSTION AND GASIFICATION OF LIQUID FUELS IN FLUIDIZED BEDS

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Abstract - Two mathematical models to allow computations of chemical species production or consumption rates by heterogeneous reactions taking place during combustion and gasification of liquid fuels sprayed on or injected into fluidized beds of solid particles are proposed. The possibilities envisaged here are called: the CIP (Coated Inert Particles) and the CSP (Coke Shell Particle) models. The former assumes that the injected liquid fuel immediately coats the fluidized inert particles in the bed and then goes through pyrolysis, combustion and gasification reactions. The latter presumes that the liquid fuel drops go through fast pyrolysis before meeting any inert particles and the remaining coke hollow particles react with gases in the bed. Analytical solutions for various geometries of the inert particles in the bed are presented. The work does not include the governing equations which constitute the whole mathematical model of fluidized-bed reactors. Such can be found elsewhere. The present work concentrates only on the theoretical aspects. Experimental tests would allow verification if they properly represent the processes of liquid consumption during combustion and gasification processes consuming liquid fuels in fluidized beds and which model would better fit each individual situation.

Keywords: Liquid Fuels, Combustion, Gasification, Mathematical Models, Fluidized-Bed.

INTRODUCTION

Fluidized-Bed technology has been successfully applied for cases of solid fuels as energy sources. The various advantages of fluidized beds, either bubbling, circulating, or entrained over more conventional combustion and gasification techniques are listed elsewhere (Basu, 2016; Kunii and Levenspiel, 1991; Kunii and Levenspiel, 1997; Geldart, 1986; de Souza-Santos, 1987; de Souza-Santos, 2010).

Fluidized beds have been particularly useful when dealing with high-moisture biomasses, municipal solid residues, high-ash coals and other low heating-value fuels (de Souza-Santos, 2010; Muskala et al., 2011).

During the years, many models have been developed to allow predictions of the behavior of existing units as well and optimizations of future ones. The list of those is too extensive, but many are described or listed in reviews (Gomez-Barea and Leckner, 2010; Philippsen et al., 2015; Alagoz, 2006;

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Saraiva et al., 1993). Nonetheless, no model has been found in the literature including the alternative of liquid fuel feeding into fluidized beds.

The present development

An existing simulation program (www.csfmb.com) has been validated (de Souza-Santos, 1987, 1989, 1994a, 1994b, 2007, 2008, 2009, 2010; Rabi and de Souza-Santos, 2003, 2004, 2008; Krzywanski et al., 2016; Englebrecht et al., 2011) and used in studies involving various possibilities and consuming many fuels, including low-quality ones (Muskala et al., 2011; de Souza-Santos, 1989, 1994a, 1994b, 2007, 2008, 2009, 2010, 2015; Rabi and de Souza-Santos, 2003, 2004, 2008; Krzywanski et al., 2016; Englebrecht et al., 2011; de Souza-Santos and Chaves, 2012a, 2012b, 2012c; de Souza-Santos and Ceribeli, 2012, 2013; de Souza-Santos and Beninca, 2014; de Souza-Santos and Lima, 2015; de Souza-Santos et al., 2015).

In many situations, fluidized beds require inert solids, such as sand or alumina, as temperature regulator and to allow more stable fluidization (Basu, 2016; Kunii and Levenspiel, 1991; Kunii and Levenspiel, 1997; Geldart, 1986; de Souza-Santos, 1987; de Souza-Santos, 2010). Ash particles, detached from the feeding solid fuel, can replace part or even the total amount of that inert material.

In addition to solid fuels, liquids or slurries are also an important segment of the spectrum found in industry. Among them there are heavy or viscous oils, whose combustion in pulverized form is cumbersome. Furthermore, several works have explored the application of residual hydrocarbon to enrich low heating value solid fuels to allow their ignition, as well as improve the combustion or gasification processes (Breault, 2010). Amid those, glycerol has shown particular interest since it is a byproduct of biodiesel production, which has increased substantially in many countries (Leonetia et al., 2012; Wei et al., 2011; Sricharoenwchaikul and Atong, 2012; Manara and Zabanioutou, 2016; Czernichowski, 2009; Fosso-Kankeu et al., 2015; Maintinguer et al., 2015; Pagliaro and Rossi, 2010). For instance, just the Brazilian output should reach 4.1 million m³ in 2016 (Barros, 2015). Since glycerol represents around 11% of biodiesel production, its rate of generation would also increase fast in the coming years (Dasari et al., 2005; Schultz et al., 2014).

An alternative for the utilization of those liquid fuels is their injection into fluidized bed boilers or gasifiers.

BASIC MODELS

The following possibilities can be visualized:

- As the liquid fuel enters the fluidized bed, it immediately coats the inert solid particles. Then, the fuel goes through pyrolysis or devolatilization and the resulting coke layers remain on the inert particles. Then, those layers are attacked by gases. This model is called here CIP (Coated Inert Particle) and the situation is illustrated by Figure 1. The Appendix describes how it can be applied for each situation where the supporting solid has a particular basic shape, i.e., planar or flat, cylindrical, or spherical.
- As the liquid fuel is sprayed into the bed, the drops go through pyrolysis before having the opportunity of meeting any inert particle. A hollow coke shell forms from each fuel drop after the volatiles escape from its interior through small holes in the respective shell. Then, the remaining shell of that hollow sphere of coke reacts with the gases. The average size among the spheres is assumed to be the same as the average drop size in the original sprayed fuel. This model is called here CSP (Coke Shell Particle) and the situation is illustrated by Figure 2.

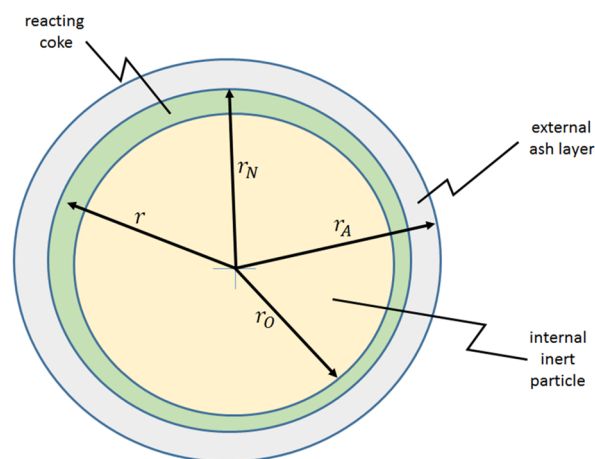


Figure 1. Scheme for the CIP model

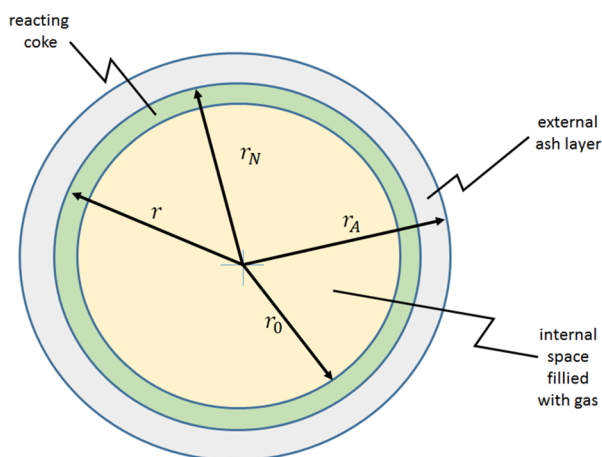


Figure 2. Scheme for the CSP model.

Before describing the mathematical models, it is important to stress that the present work assumes isothermal conditions in the layer of fuel and inert particles. The local temperature of particles, as well as temperature, pressure, and composition of the surrounding gas, should be given by a comprehensive model for fluidized-bed equipment. The governing equations that constitute the mathematical model of fluidized-bed reactors can be found elsewhere (de Souza-Santos, 2010). The only objective here is to present the equations proposed for the reaction rates between gases and the liquid fuel injected into the reactor with fluidized inert solid particles.

The treatment for a single heterogeneous reaction i , in which a chemical component j of the surrounding gas is consumed or produced, has been presented by de Souza-Santos (2010). In any case, the fundamental equation for conservation of species leads to

$$\nabla^2 y = \Phi^2 y^n \quad (1)$$

The Laplacian operator is generalized as:

$$\nabla^2 = x^{-p} \frac{d}{dx} \left(x^p \frac{d}{dx} \right) \quad (2)$$

the coefficient p takes the following possible values: 0 for plane geometry, 1 for cylindrical, and 2 for spherical. Here:

$$x = \frac{r}{r_A} \quad (3)$$

$$y = \frac{\tilde{\rho}_j - \tilde{\rho}_{j,eq}}{\tilde{\rho}_{j,\infty} - \tilde{\rho}_{j,eq}} \quad (4)$$

The Thiele coefficient is given by:

$$\Phi = r_A \left[\frac{k_i (\tilde{\rho}_{j,\infty} - \tilde{\rho}_{j,eq})^{n-1}}{D_{j,N}} \right]^{1/2} \quad (5)$$

On the above, it has been assumed that all reaction rates could be written as:

$$\tilde{r}_i = k_i (\tilde{\rho}_j - \tilde{\rho}_{j,eq})^n \quad (6)$$

which is valid for most of the combustion and gasification reactions. For those, the reaction order n varies between 0 and 2. However, the main cases of carbon-oxygen and carbon-water reactions-which control most of the combustion and gasification processes-follow a first order behavior. A list of several reactions found in those processes as well their kinetic coefficients are presented elsewhere (de Souza-Santos, 2010).

The basic equations to allow computation of the CIP and CSP models are present below.

Coated Inert Particle (CIP) Model

Figure 1 illustrates the CIP model. The inert particle, coated by a coke layer, may present three basic shapes: plane (in the case of chips), cylindrical (in the case of pellets or fibers), and spherical or almost spherical. As detailed in the Appendix, the solutions can be condensed into a single formula for the rate of consumption or production of component j by reaction i as

$$r_j = \frac{1}{r_A} \frac{\tilde{\rho}_{j,\infty} - \tilde{\rho}_{j,eq}}{\sum_{k=1}^3 U_k} \quad (7)$$

The sum that appears in the denominator represents the three resistances in series for mass transfers of chemical species j that depend on the inert particle original shape. Table 1 summarizes the various possibilities. The first parameter U_1 represents the resistance to the mass transfer at the gas boundary layer, U_2 the resistance at the ash layer, and the U_3 the combined resistances of reacting gas mass transfer through the reactive coke layer and its respective chemical reaction with the coke material. The various resistances for the basic geometries are summarized at Table 1. An example of deduction is shown in the Appendix.

Table 1. Formulas to compute the mass transfer resistances in the case of CIP model.

Shape	Resistance		
	U1	U2	U3 (*)
Plate	$\frac{1}{N_{Sh} D_{j,G}}$	$\frac{1-a}{D_{j,A}}$	$\frac{1}{\Phi D_{j,N}} \frac{C_a C_b - S_a S_b}{S_a C_b - C_a S_b}$
Cylinder	$\frac{1}{N_{Sh} D_{j,G}}$	$-\frac{\ln(a)}{D_{j,A}}$	$\frac{1}{a \Phi D_{j,N}} \frac{I_0(a \Phi) K_1(b \Phi) + I_1(b \Phi) K_0(a \Phi)}{I_1(a \Phi) K_1(b \Phi) - I_1(b \Phi) K_1(a \Phi)}$
Sphere	$\frac{1}{N_{Sh} D_{j,G}}$	$\frac{1-a}{a D_{j,A}}$	$\frac{1}{a D_{j,N}} \frac{(S_b - b \Phi C_b) C_a - (C_b - b \Phi S_b) S_a}{(C_b - b \Phi S_b) (S_a - a \Phi C_a) - (S_b - b \Phi C_b) (C_a - a \Phi S_a)}$

(*) Here: $S_a = \sinh(a \Phi)$, $S_b = \sinh(b \Phi)$, $C_a = \cosh(a \Phi)$, $C_b = \cosh(b \Phi)$

Coke Shell Particle (CSP) Model

Figure 2 illustrates the situation for the CSP model. Here just the spherical shape is possible.

The first aspect to face is to estimate the radius of the internal space filled with gases.

The original mass of the droplet is given by

$$m_\ell = \frac{4\pi}{3} r_A^3 \rho_\ell \quad (8)$$

On the other hand, the mass of the coke before the formation of ash over it, is provided by

$$m_c = \frac{4\pi}{3} (r_A^3 - r_0^3) \rho_c \quad (9)$$

However,

$$m_c = m_\ell (1 - f_V - f_M) = m_\ell f \quad (10)$$

Therefore,

$$r_0 = r_A \left[1 - \frac{\rho_\ell f}{\rho_c} \right]^{1/3} \quad (11)$$

The deduction for the resistances are presented in the Appendix. These resistances can be employed in Eq. (7) to compute the rate of consumption or production of gas component j by reaction i .

DISCUSSION

According to Equation 58 of the Appendix, in the case of CSP model, if no mass transfer at the internal cavity surface takes place (i.e., $N_2 = 0$), the parameter equals the variable a and the resistance forms reproduce the CIP case for spherical geometry.

Another interesting aspect of that case can be appreciated by noticing that the parameter g_j (Eq. 45 in the Appendix) is a function of the average

concentration inside the cavity. At the beginning of cavity formation, the concentration would be equal to those obtained from the pyrolysis. After a while, the composition tends to equalize the concentration of the equilibrium atmosphere in which the particle is immersed. Therefore, for long exposure times, g_j would tend to zero. This situation reproduces the case where $N_2 = 0$.

CONCLUSIONS

The possibility of using the fluidized-bed technique for combustion and gasification of liquid fuels is known. In those cases, the liquid is sprayed over or injected into the bed where inert solid is fluidized.

The adaptation of existing simulation models to such situations required methods to compute the kinetics for heterogeneous reactions. To allow that, two possible approaches are proposed here: the CIP (Coated inert Particle) Model and the CSP (Coke-Shell Particle) Model. The work introduces the analytical solutions for those models, as well as for cases of different basic shapes of inert particles present in the bed.

The present proposals are theoretical. Future publications might confirm the deductions made here and which model would better represent the process in each situation.

APPENDIX

CIP Model for Plane Geometry

Figure 3 illustrates the situation where the slab or chip is assumed to have a thickness much smaller than any other dimension. Therefore, all variations occur in the r direction, which is normal to the surface with largest area.

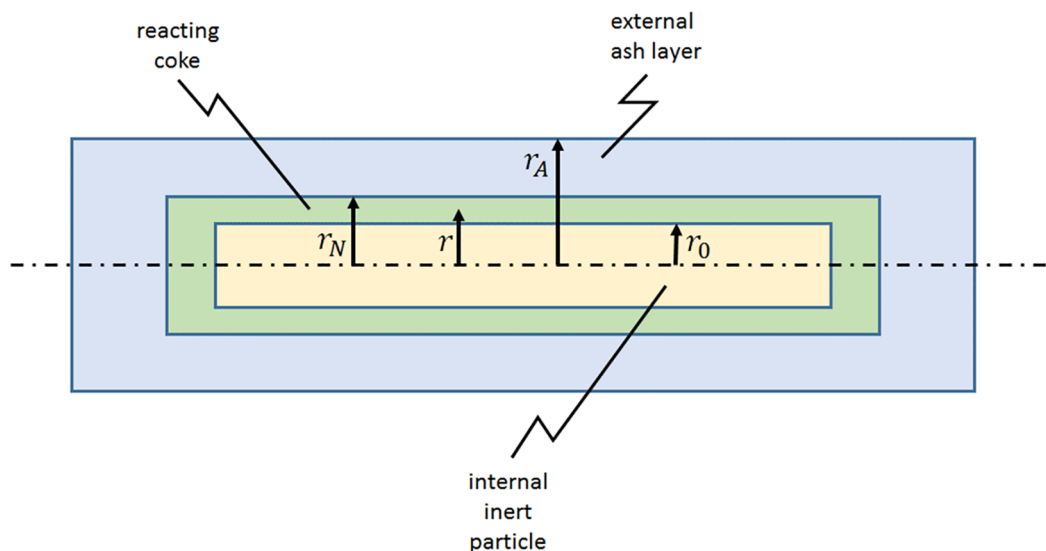


Figure 3. CIP model for planar geometry.

Using $p = 0$ in Equation (1), it is possible to write

$$\frac{d^2 y}{dx^2} = \Phi^2 y \quad (12)$$

For the ash layer where no reaction takes place, it leads to

$$\frac{dy}{dx} = A_1, \quad a \leq X \leq 1 \quad (13)$$

and

$$y = A_1 x + B_1, \quad a \leq X \leq 1 \quad (14)$$

where the parameter a is given by:

$$a = \frac{r_N}{r_A} \quad (15)$$

One boundary condition can be set for the external surface, or at $x=1$, where continuity imposes that the mass transfer by diffusion of the reacting gas j equals the mass transfer by convection, or:

$$D_{j,G} \frac{d\tilde{\rho}_j}{dr} \Big|_{r=r_A^+} = D_{j,A} \frac{d\tilde{\rho}_j}{dr} \Big|_{r=r_A^-} = \beta_G (\tilde{\rho}_{j,\infty} - \tilde{\rho}_{j,surf}) \quad (16)$$

or

$$y'(1) = N_{Sh} [1 - y(1)] \frac{D_{j,G}}{D_{j,A}} = N_1 [1 - y(1)] \quad (17)$$

where the Sherwood number is:

$$N_{Sh} = \frac{\beta_G r_A}{D_{j,G}} \quad (18)$$

and:

$$N_1 = N_{Sh} \frac{D_{j,G}}{D_{j,A}} \quad (19)$$

It should be noticed that the coefficient D_j is the diffusivity of component j into the phase in which the process takes place. If that phase is the particle core, or nucleus, the parameter is called the "effective" diffusivity of j in that porous structure, which is represented by $D_{j,N}$. A similar notation will be used for the diffusivity of j through the shell of inert porous solid that coats the core, or $D_{j,A}$. For the boundary layer of gas, which surrounds the particle, the value is the average diffusivity of j through the gas mixture that constitutes the layer, or $D_{j,G}$. As it was shown long ago by Walker et al. (1959), the values for effective diffusivity can be correlated to the gas-gas diffusivity $D_{j,G}$.

From (12) and (13) in (17) it is possible to write

$$B_1 = 1 - \frac{1 + N_1}{N_1} A_1 \quad (20)$$

Therefore,

$$y = A_1 \left[x - \frac{1 + N_1}{N_1} \right] + 1, \quad a \leq X \leq 1 \quad (21)$$

In the reacting coke layer, Eq. (12) becomes a Bessel equation and its solution can be written as:

$$y = A_2 \sinh(x\Phi) + B_2 \cosh(x\Phi), \quad b \leq X \leq a \quad (22)$$

Where:

$$b = \frac{r_0}{r_A} \quad (23)$$

A boundary condition can be found at $x = b$. As the inert material is impermeable to the reacting gas, the mass transfer is zero at that interface, or

$$\left. \frac{dy}{dx} \right|_{x=b} = 0 \quad (24)$$

Therefore, Eq. (22) becomes:

$$y = B_2 \left[\frac{\cosh(x\Phi) - \tanh(b\Phi)}{\sinh(x\Phi)} \right], b \leq X \leq a \quad (25)$$

The other condition comes from continuity of the mass transfer at the coke-ash interface, or:

$$D_{j,N} \left. \frac{dy}{dx} \right|_{x=a^-} = D_{j,A} \left. \frac{dy}{dx} \right|_{x=a^+} \quad (26)$$

Equations (13) and (25) lead to:

$$B_2 = A_1 \frac{D_{j,A}}{D_{j,N} \Phi} \left[\frac{\sinh(a\Phi) - \tanh(b\Phi)}{\cosh(a\Phi)} \right]^{-1} \quad (27)$$

Therefore,

$$y = A_1 \frac{D_{j,A}}{\Phi D_{j,N}} \frac{\cosh(x\Phi) - \tanh(b\Phi) \sinh(x\Phi)}{\sinh(a\Phi) - \tanh(b\Phi) \cosh(a\Phi)}, \quad b \leq X \leq a \quad (28)$$

In addition, the concentrations match at that interface or $y(a^-) = y(a^+)$. Thus, the above equation can be combined with Eq. (21) to give:

$$A_1 = \frac{1}{\frac{D_{j,A}}{D_{j,N}} \xi + \frac{1 + N_1}{N_1} - a} \quad (29)$$

where:

$$\xi = \frac{1}{\Phi} \frac{\cosh(a\Phi) - \tanh(b\Phi) \sinh(a\Phi)}{\sinh(a\Phi) - \tanh(b\Phi) \cosh(a\Phi)} \quad (30)$$

The rate of consumption or production of component j is given by the mass transfer of that component at the external layer, or:

$$r_j = D_{j,A} \left. \frac{d\tilde{\rho}_j}{dr} \right|_{r=r_A} = \frac{D_{j,A} (\tilde{\rho}_{j,\infty} - \tilde{\rho}_{j,eq})}{r_A} \left. \frac{dy}{dx} \right|_{x=1} \quad (31)$$

Finally, using Eq. (13), it is possible to obtain the resistances listed for the plane geometry as shown in Table 1.

The deductions for other geometry ($p = 1$ and $p = 2$) follow the same path.

The values of the parameters a (Eq. 15) and b (Eq. 23), or dimensionless variables, need to be addressed. It is easy to show that they can be computed by:

$$a = \frac{d_{P,inert} + 2f\delta}{d_{P,inert} + 2\delta} \quad (32)$$

and

$$b = \frac{d_{P,inert}}{d_{P,inert} + 2\delta} \quad (33)$$

where f represents the fraction of the fixed-carbon, originally in the feeding fuel, which is converted into gases, and d is the film thickness. This thickness can be easily computed by assuming that all particles present in the bed are equally and uniformly coated by the feeding liquid. Given the very high circulation rates of particles in a bubbling or circulating fluidized bed, this should not be very far from reality.

CSP Model

From Equations (1) and (2)

$$\frac{dy}{dx} = A_1 x^{-2} \quad (34)$$

$$y = -A_1 x^{-1} + B_1, a \leq X \leq 1 \quad (35)$$

The boundary condition (17) leads to

$$B_1 = 1 - \frac{1 - N_1}{N_1} A_1 \quad (36)$$

where N_1 is given by Eq. (19).

For the coke reacting layer, the following can be written

$$x^2 y'' + 2xy' - x^2 \Phi^2 y = 0 \quad (37)$$

and the solution of that Bessel equation is

$$y = A_2 \frac{\sinh(x\Phi)}{x} + B_2 \frac{\cosh(x\Phi)}{x}, b \leq X \leq a \quad (38)$$

From the continuity for the mass transfer at the coke-ash interface (Eq. 26), it is possible to write:

$$\frac{D_{j,N}}{D_{j,A}} A_1 + A_2 [\sinh(a\Phi) - a\Phi \cosh(a\Phi)] + B_2 [\cosh(a\Phi) - a\Phi \sinh(a\Phi)] = 0 \quad (39)$$

The following comes from the continuity or equality of concentration at the two sides of the interface:

$$A_1 \left(\frac{1}{a} + \frac{1 - N_1}{N_1} \right) + A_2 \frac{\sinh(a\Phi)}{a} + B_2 \frac{\cosh(a\Phi)}{a} = 1 \quad (40)$$

At the internal surface of the shell (coke-cavity-gas), the following is required:

$$D_{j,N} \frac{d\tilde{\rho}_j}{dr} \Big|_{r=r_0^+} = D_{j,G} \frac{d\tilde{\rho}_j}{dr} \Big|_{r=r_0^-} = \beta_{cav} (\tilde{\rho}_{j,r=r_0} - \tilde{\rho}_{j,cav}) \quad (41)$$

or:

$$y'(b) = N_{Sh,cav} [y(b) + \gamma] \frac{D_{j,G}}{D_{j,N}} = N_2 [y(b) + \gamma] \quad (42)$$

where:

$$N_{Sh,cav} = \frac{\beta_{cav} r_0}{D_{j,G}} \quad (43)$$

and

$$N_2 = N_{Sh,cav} \frac{D_{j,G}}{D_{j,N}} \quad (44)$$

$$\gamma_j = \frac{\tilde{\rho}_{j,cav} - \tilde{\rho}_{j,eq}}{\tilde{\rho}_{j,\infty} - \tilde{\rho}_{j,eq}} \quad (45)$$

The combination of above equations leads to:

$$A_2 \left[\left(\frac{N_2}{b} + \frac{1}{b^2} \right) \sinh(b\Phi) - A\Phi \frac{\cosh(b\Phi)}{b} \right] + B_2 \left[\left(\frac{N_2}{b} + \frac{1}{b^2} \right) \cosh(b\Phi) - \Phi \frac{\sinh(b\Phi)}{b} \right] = N_2 \gamma_j \quad (46)$$

or

$$A_2 [(1 + N_2 b) S_b - \Phi b C_b] + B_2 [(1 + N_2 b) C_b - \Phi b S_b] = N_2 \gamma_j b^2 \quad (47)$$

The continuity of mass transfer rate at the coke-ash interface leads to:

$$A_2 [-S_a + \Phi a C_a] + B_2 [-C_a + \Phi a S_a] = \frac{D_{j,A}}{D_{j,N}} A_1 \quad (48)$$

Equality of concentration at the coke-ash interface, to:

$$A_2 S_a + B_2 C_a = -A_1 \left(1 + a \frac{1 - N_1}{N_1} \right) + a \quad (49)$$

A_2 , and B_2 can be eliminated from the three above equations in order to obtain A_1 as:

$$A_1 = \left[\frac{(a C_1 - S_a N_2 \gamma_j b^2)(C_1 C_4 - C_2 C_3) +}{N_2 \gamma_j b^2 C_3 (C_1 C_a - C_2 S_a)} \right] / \left[\left(1 + a \frac{1 - N_1}{N_1} \right) C_1 (C_1 C_4 - C_2 C_3) + \frac{D_{j,A}}{D_{j,N}} C_1 (C_1 C_a - C_2 S_a) \right] \quad (50)$$

where:

$$C_1 = S_b + N_2 b S_b - \Phi b C_b \quad (51)$$

$$C_2 = C_b + N_2 b C_b - \Phi b S_b \quad (52)$$

$$C_3 = \Phi a C_a - S_a \quad (53)$$

$$C_4 = \Phi a S_a - C_a \quad (54)$$

Finally,

$$U_1 = \frac{a}{N_{Sh} D_{j,G}} \frac{1}{\omega} \quad (55)$$

$$U_2 = \frac{1 - a}{D_{j,A}} \frac{1}{\omega} \quad (56)$$

$$U_3 = \frac{\Xi}{D_{j,N}} \frac{1}{\omega} \quad (57)$$

Here

$$\omega = a - \frac{N_2 b^2 \gamma_j}{C_1} (S_a - C_3 \Xi) \quad (58)$$

with

$$\Xi = \frac{C_1 C_a - C_2 S_a}{C_1 C_4 - C_2 C_3} \quad (59)$$

NOMENCLATURE

a, A, b, B, C - parameters (dimensionless)
 C_a, C_b - see observation under Table 1 (dimensionless)
 d_p - particle diameter or thickness in the cases of slabs
 D_j - average equivalent or effective diffusivity of chemical species j (the second subscript indicates the medium) ($\text{m}^2 \text{s}^{-1}$)
f - fractional conversion of fixed-carbon originally in the fuel (dimensionless)
I - Modified Bessel function of the first kind (subscript indicates order)
 k_i - rate coefficient of reaction i [$\text{s}^{-1} (\text{kmol}^{-1} \text{m}^3)^n$]
K - Modified Bessel function of the second kind (subscript indicates order)
m - mass (kg)
n - reaction order
N - parameter (dimensionless)
 N_{sh} - Sherwood number
p - parameter to indicate the geometrical form
r - radial co-ordinate (m). In cases of slabs or chips, it is the distance between the centerline of the slab and the outer surface (with the largest area) of the ash layer (m).
 \tilde{r}_i''' - reaction rate ($\text{kmol m}^{-3} \text{s}^{-1}$)
 \tilde{r}_i'' - reaction rate based on the external area of the particle ($\text{kmol m}^{-2} \text{s}^{-1}$)
 S_a, S_b - see observation under Table 1 (dimensionless)
U - resistance to mass transfer (s m^{-2})
x - dimensionless co-ordinate
y - dimensionless concentration of reacting gas

Greek Letters

β - mass transfer coefficient (m s^{-1})
 γ - dimensionless concentration

δ - film thickness (m)
 Φ - Thiele modulus or coefficient (dimensionless)
 ρ - density (kg m^{-3})
 $\tilde{\rho}_j$ - molar concentration of the reacting chemical species j (kmol m^{-3})
 ξ - parameter (dimensionless)
 ω - parameter (dimensionless)
 Ξ - parameter (dimensionless)

Subscripts

A - ash
c - coke
Eq - at equilibrium condition
G - gas phase
i - chemical reaction number
j - chemical component
l - liquid
M - moisture in the original fuel
N - active or reacting coke layer
O - original or internal
V - volatile in the original fuel
 ∞ - at conditions in the surrounding gas and far from the reacting particle

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