Combustion Model of Packed Particles

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1 Introduction

2 Mathematical Model

2.1 Governing Equation

Consider the following radially symmetric cylindrical model. At a distance x consider an infinitesimal slice of dx.

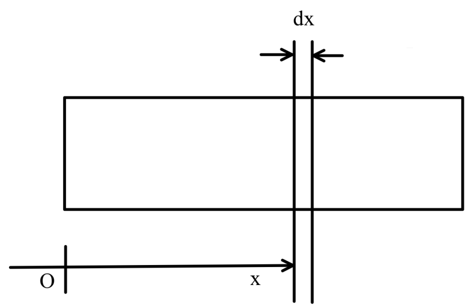

Figure 1: Energy balance for an infinitesimal slice

The governing equation from energy balance for the infinitesimal slice is given by

$$\rho_m C_{p,m} \frac{\partial T}{\partial t} = \lambda_m \frac{\partial^2 T}{\partial x^2} + \frac{\rho_m Q_r \dot{\omega}}{(MW)_{prod}} - \frac{4}{D} \left[h \left(T - T_a \right) + \varepsilon \sigma \left(T^4 - T_a^4 \right) \right] \tag{1}$$

The boundary conditions are

- $T \left(t, x = 0 \right) = T_f$
- $\frac{\partial T}{\partial x}|_{t, x=L} = 0$

The initial condition is $T \left(t = 0, x \right) = T_u$

2.2 Discretization

2.2.1 Temperature Predictor Step

$$\rho_m C_{p,m} \frac{\hat{T}_i - T_i^{n/k}}{\Delta t} = \lambda_m \left\{ \frac{\hat{T}_{i+1} - 2\hat{T}_i + \hat{T}_{i-1}}{\left(\Delta x\right)^2} \right\}$$

$$\Rightarrow \left\{ \frac{\lambda_m}{\left(\Delta x\right)^2} \right\} \hat{T}_{i+1} - \left\{ 2 \frac{\lambda_m}{\left(\Delta x\right)^2} + \frac{\rho_m C_{p,m}}{\Delta t} \right\} \hat{T}_i + \left\{ \frac{\lambda_m}{\left(\Delta x\right)^2} \right\} \hat{T}_{i-1} = - \left\{ \frac{\rho_m C_{p,m}}{\Delta t} \right\} T_i^{n/k} \tag{2}$$

2.2.2 Conversion Corrector Step

$$\eta_i^{n/k+1} = \frac{\eta_i^{n/k} + k\left(\hat{T}\right)\Delta t}{1 + k\left(\hat{T}\right)\Delta t} \tag{3}$$

2.2.3 Temperature Corrector Step

$$\begin{aligned}
\rho_m C_{p,m}\frac{T_i^{n/k+1} - \hat{T}_i}{\Delta t} &= \frac{\rho_m Q_r}{(MW)_{prod}} k\left(T_i^{n/k+1}\right)\left(1 - \eta_i^{n/k+1}\right) - \frac{4h}{D}\left(T_i^{n/k+1} - T_a\right) - \frac{4\varepsilon\sigma}{D}\left\{\left(T_i^{n/k+1}\right)^4 - T_a^4\right\} \\
&= \frac{\rho_m Q_r}{(MW)_{prod}}\left(1 - \eta_i^{n/k+1}\right)\left\{k\left(\hat{T}_i\right) + k'\left(\hat{T}_i\right)\left(T_i^{n/k+1} - \hat{T}_i\right)\right\} \\
&\quad - \frac{4h}{D}\left(T_i^{n/k+1} - T_a\right) - \frac{4\varepsilon\sigma}{D}\left\{\hat{T}_i^4 + 4\hat{T}_i^3\left(T_i^{n/k+1} - \hat{T}_i\right) - T_a^4\right\}
\end{aligned}$$

$$T_i^{n/k+1} = \frac{\frac{\rho_m C_{p,m}}{\Delta t}\hat{T}_i + \frac{\rho_m Q_r}{(MW)_{prod}}\left(1 - \eta_i^{n/k+1}\right)\left\{k\left(\hat{T}_i\right) - k'\left(\hat{T}_i\right)\hat{T}_i\right\} + \frac{4h}{D}T_a + \frac{4\varepsilon\sigma}{D}\left(3\hat{T}_i^4 + T_a^4\right)}{\frac{\rho_m C_{p,m}}{\Delta t} + \frac{\rho_m Q_r}{(MW)_{prod}}\left(1 - \eta_i^{n/k+1}\right)k'\left(\hat{T}_i\right) + \frac{4h}{D} + 16\frac{\varepsilon\sigma}{D}\hat{T}_i^3} \tag{4}$$

3 Thermophysical Properties

3.1 Thermal Conductivity λ_m

3.1.1 Maxwell - Eucken - Bruggeman Model

A combination of Maxwell - Eucken and Bruggeman models is used to predict the thermal conductivity of the packed particles degassed with a fluid.

$$\lambda_m\left(\phi_p, \alpha_{p,ME}, \lambda_p, \lambda_f\right) = \frac{X + \sqrt{X^2 + 2\lambda_p\lambda_f}}{2} \tag{5}$$

$$X = \left(2\lambda_p - \lambda_f\right)\phi_p\left(1 - \alpha_{p,ME}\right) + \left(2\lambda_f - \lambda_p\right)\phi_f\left(\frac{2\phi_f + 2\phi_p\alpha_{p,ME} - 1}{2\phi_f}\right)$$

where -

- λ_p is the thermal conductivity of the particle
- λ_f is the thermal conductivity of the fluid
- ϕ_p is the volume fraction of the particles
- ϕ_f is the volume fraction of the fluid
- $\alpha_{p,ME}$ is the volume fraction of the particles with structure represented by Maxwell-Eucken

3.1.2 Thermal Conductivity of a Coated Spherical Particle

$$\lambda_p\left(\lambda_c, \lambda_s, R, r\right) = \frac{\lambda_c^2 R}{(r - R)\left[2\lambda_c \ln a - 2\lambda_s \ln a - \left(\frac{\lambda_c^2}{\lambda_s}\right)\right] + r\lambda_c} \tag{6}$$

$$a = \frac{b - \lambda_c R}{b - \lambda_c\left(R - r\right)}$$

$$b = 2\left(R - r\right)\lambda_s + 2r\lambda_c$$

where -

- λ_c is the thermal conductivity of the core material
- λ_s is the thermal conductivity of the shell material
- R is the outer radius (core + shell)
- r is the inner radius (core)

3.2 Density ρ_m

3.2.1 Density of Fluid - Packed Particles Mixture

$$\rho_m\left(\phi_p, \rho_p, \rho_f\right) = \phi_p \rho_p + \left(1 - \phi_p\right) \rho_f \tag{7}$$

where -

- ρ_p is the density of the particle
- ρ_f is the density of the fluid
- ϕ_p is the volume fraction of particles

3.2.2 Density of Coated Spherical Particle

$$\rho_p\left(\rho_c, \rho_s, R, r\right) = \frac{r^3 \rho_c + \left(R^3 - r^3\right) \rho_s}{R^3} \tag{8}$$

where -

- ρ_c is the density of the core material
- ρ_s is the density of the shell material

3.3 Specific Heat Capacity $C_{p,m}$

3.3.1 Specific Heat Capacity of Fluid - Packed Particle Mixture

$$C_{p,m}\left(\phi_p, \rho_p, \rho_f, C_{p,p}, C_{p,f}\right) = \frac{\phi_p \rho_p C_{p,p} + \left(1 - \phi_p\right) \rho_f C_{p,f}}{\phi_p \rho_p + \left(1 - \phi_p\right) \rho_f} \tag{9}$$

where -

- $C_{p,p}$ is the specific heat capacity of the particles
- $C_{p,f}$ is the specific heat capacity of the fluid

3.3.2 Specific Heat Capacity of Coated Spherical Particle

$$C_{p,p}\left(\rho_c, \rho_s, C_{p,c}, C_{p,s}, R, r\right) = \frac{r^3 \rho_c C_{p,c} + \left(R^3 - r^3\right) \rho_s C_{p,s}}{r^3 \rho_c + \left(R^3 - r^3\right) \rho_s} \tag{10}$$

where -

- $C_{p,c}$ is the specific heat capacity of the core material
- $C_{p,s}$ is the specific heat capacity of the shell material

3.4 Properties of Packed Pellets of Ni-Coated Al Particles degassed with Ar

3.4.1 Preheat Zone

All thermophysical properties are evaluated at average temperature encountered in the Preheat Zone.

- $\lambda_{m,P} = \lambda_m \left(\phi_p, \alpha_{p,ME}, \lambda_{p,P}, \lambda_{Ar,P}\right)$
- $\rho_{m,P} = \rho_m \left(\phi_p, \rho_{p,P}, \rho_{Ar,P}\right)$
- $C_{p,m,P} = C_{p,m} \left(\phi_p, \rho_{p,P}, \rho_{Ar,P}, C_{p,p,P}, C_{p,Ar,P}\right)$

Properties of the Ni-coated Al particles in the preheat zone

- $\lambda_{p,P} = \lambda_p \left(\lambda_{Al,P}, \lambda_{Ni,P}, R, r\right) = 137\ W/m-K$
- $\rho_{p,P} = \rho_p \left(\rho_{Al,P}, \rho_{Ni,P}, R, r\right) = 5430\ kg/m^3$
- $C_{p,m,P} = C_{p,p} \left(\rho_{Al,P}, \rho_{Ni,P}, C_{p,Al,P}, C_{p,Ni,P}, R, r\right) = 613\ J/kg-K$
- $r = 32.5\mu m$
- $R = 39.5\mu m$

	$\lambda\,(W/m-K)$	$\rho\left(kg/m^3\right)$	$C_p\,(J/kg-K)$
Ar	0.016	0.89	520
Al	220	2700	1060
Ni	66	8908	440

Table 1: Properties of Pure Substances in the Preheat Zone

3.4.2 Post Combustion Zone

All thermophysical properties are evaluated at average temperature encountered in the Post Combustion Zone.

- $\lambda_{m,PC} = \lambda_m \left(\phi_p, \alpha_{p,ME}, \lambda_{NiAl,PC}, \lambda_{Ar,PC}\right)$
- $\rho_{m,PC} = \rho_m \left(\phi_p, \rho_{NiAl,PC}, \rho_{Ar,PC}\right)$
- $C_{p,m,PC} = C_{p,m} \left(\phi_p, \rho_{NiAl,PC}, \rho_{Ar,PC}, C_{p,NiAl,PC}, C_{p,Ar,PC}\right)$

	$\lambda\,(W/m-K)$	$\rho\left(kg/m^3\right)$	$C_p\,(J/kg-K)$
Ar	0.055	0.37	520
NiAl	115	5900	717

Table 2: Properties of Pure Substances in the Post Combustion Zone

3.4.3 Reaction Zone

All thermophysical properties are evaluated at average temperature encountered in the Reaction Zone.

- $\lambda_{m,R} = \lambda_m \left(\phi_p, \alpha_{p,ME}, \lambda_{p,R}, \lambda_{Ar,R}\right)$
- $\rho_{m,R} = \rho_m \left(\phi_p, \rho_{p,R}, \rho_{Ar,R}\right)$
- $C_{p,m,R} = C_{p,m} \left(\phi_p, \rho_{p,R}, \rho_{Ar,R}, C_{p,p,R}, C_{p,Ar,R}\right)$

The mean properties of the reactants and the products is considered for the particles.

- $\lambda_{p,R} = 0.5\left(\lambda_p\left(\lambda_{Al,R}, \lambda_{Ni,R}, R, r\right) + \lambda_{NiAl,R}\right)$
- $\rho_{p,R} = 0.5\left(\rho_p\left(\rho_{Al,R}, \rho_{Ni,R}, R, r\right) + \rho_{NiAl,R}\right)$
- $C_{p,m,R} = 0.5\left(C_{p,p}\left(\rho_{Al,R}, \rho_{Ni,R}, C_{p,Al,R}, C_{p,Ni,R}, R, r\right) + C_{p,NiAl,R}\right)$
- $\lambda_p\left(\lambda_{Al,R}, \lambda_{Ni,R}, R, r\right) = 108\ W/m-K$
- $\rho_p\left(\rho_{Al,R}, \rho_{Ni,R}, R, r\right) = 5430\ kg/m^3$
- $C_{p,p}\left(\rho_{Al,R}, \rho_{Ni,R}, C_{p,Al,R}, C_{p,Ni,R}, R, r\right) = 760\ J/kg-K$
- $r = 32.5\mu m$
- $R = 39.5\mu m$

	$\lambda\,(W/m-K)$	$\rho\,(kg/m^3)$	$C_p\,(J/kg-K)$
Ar	0.055	0.37	520
Al	130	2700	1176
Ni	80	8908	670
NiAl	115	5900	717

Table 3: Properties of Pure Substances in the Reaction Zone

4 Kinetics

4.1 Physics

For a model reaction

$$A \longrightarrow B$$

Define the rate of change in conversion η

$$\omega = \frac{d\eta}{dt} \tag{11}$$

Following a first order reaction rate model

$$\omega(T,\eta) = k(T) \cdot (1-\eta) \tag{12}$$

Using Arrhenius Rate Law

$$k(T) = A \cdot \exp\left(-\frac{E_a}{R_u T}\right) \tag{13}$$

4.2 Discretization

Discretizing first order time derivative using backward difference scheme

$$\frac{d\eta}{dt} \approx \frac{\eta_i^n - \eta_i^{n-1}}{\Delta t} \tag{14}$$

Building implicit update equation for η

$$\frac{\eta_i^n - \eta_i^{n-1}}{\Delta t} = k\left(T_i^n\right) \cdot \left(1 - \eta_i^n\right)$$

$$\Rightarrow [1 + k(T_i^n)\,\Delta t] \cdot \eta_i^n = \eta_i^{n-1} + k(T_i^n)\,\Delta t$$

$$\Rightarrow \eta_i^n = \frac{\eta_i^{n-1} + k(T_i^n)\,\Delta t}{1 + k(T_i^n)\,\Delta t} \tag{15}$$

4.3 Combustion of Ni-coated Al Pellets

Assuming the diffusion of Al across the Ni coating as the rate dominating step, burning time is given by

$$t_b = \omega^{-1} = \frac{r^2}{cD(T)} \tag{16}$$

where r is the radius of the core, D is the diffusion coefficient, and c is the burning time constant, assumed to be six.

The diffusion coefficient as function of temperature is governed by

$$D(T) = D_0 \cdot \exp\left(-\frac{E_a}{R_u T}\right) \tag{17}$$

where $D_0 = 9.54 \times 10^{-8}\ m^2/s$ and $E_a = 26 \times 10^3\ J/mol$.

We assume at $\eta = 0$,

$$\omega|_{\eta=0} = \frac{cD}{r} = 1.76123 \times 10^{-2} \cdot \exp\left(-\frac{26 \times 10^3}{R_u T}\right) \tag{18}$$

Comparing with the Arrhenius Rate Law, $A = 1.76123 \times 10^{-2}$ and $E_a = 26 \times 10^3$ in SI units. The change in enthalpy for this reaction is $\Delta H = -118.4 \times 10^3\ J/mol$.