1 Symbol List

Table 1: Symbol list

symbol	name	unit
$k_{L,i}$	Liquid side mass transfer coefficient	$m s^{-1}$
a_L	Gas-liquid interfacial area per unit liquid volume	$m^2/m^3 = m^{-1}$
$k_{L,i}^{L}a$	Liquid side volumetric mass transfer coefficient	$m^{-1} m s^{-1} = s^{-1}$
y_i	Gas phase mole fraction of component i	_
x_i	Liquid phase mole fraction of component i	_ ,
	Gas phase mole fraction of component i at the phase boundary	_
$y_i^* \\ x_i^*$	Liquid phase mole fraction of component i at the phase boundary	_ ,
k_i^i	"Constant" describing the relationship y_i^*/x_i^* at given conditions	_
$\omega_{i,G}$	Gas phase weight fraction of component i	_
$\omega_{i,G}^*$	Gas phase weight fraction of component i at the phase boundary	_
$\omega_{i,L}$	Liquid phase weight fraction of component i	_
$\omega_{i,L}$ $\omega_{i,L}^*$	Liquid phase weight fraction of component i at the phase boundary	_
$z^{\iota,\scriptscriptstyle L}$	Reactor height	m
$ ho_L$	Total density, liquid phase	kgm^{-3}
ρ_G	Total density, gas phase	kgm^{-3}
$ \rho_S = \rho_{\rm cat} $	Catalyst density density	kgm^{-3}
$ ho_{SL}$	Slurry density	kgm^{-3}
v_G	Gas velocity	$m s^{-1}$
v_L	Liquid velocity	$m s^{-1}$
v_{SL}	Slurry velocity	$m s^{-1}$
	Gas superficial velocity	$m s^{-1}$
v_L^s	Liquid superficial velocity	$m s^{-1}$
v_{SL}^{s}	Slurry superficial velocity	$m s^{-1}$
$v_G^s \\ v_L^s \\ \frac{v_{SL}^s}{M_G} \\ \overline{M_L}$	Gas phase average molar mass	$kg kmol^{-1}$
$\overline{M_L}$	Liquid phase average molar mass	$kg kmol^{-1}$
ϵ_L	Liquid volume fraction	_
ϵ_G	Gas volume fraction	_
ϵ_S	Solid volume fraction	_
ϵ_{SL}	Slurry volume fraction	_
ϕ_L	Liquid mass fraction	_
ϕ_G	Gas mass fraction	_
ϕ_S	Solid mass fraction	_
ϕ_{SL}	Slurry mass fraction	_
$ u_i$	Stochiometric coefficient for component i	_
r_{CO}	Reaction rate in terms of CO conversion	$kmols^{-1}kg_{cat}^{-1}$
$M_{w,i}$	Molecular weight of component i	$kg kmol^{-1}$
$ ho_{cat}$	Density of catalyst	$kg_{cat} m^{-3}$
T	Temperature	K
T_G	Temperature, Gas Phase	K
T_L	Temperature, Liquid Phase	K
T_{SL}	Temperature, Slurry Phase	K
$T_{ m surr}$	Temperature, Surroundings	K
p	Pressure	Pa

Table 1: Symbol list

symbol	name	unit
p_G	Gas phase pressure	Pa
p_L	Liquid phase pressure	Pa
h	Height of dispersion	m
R	Gas constant (value: 8.314×10^3)	$J K^{-1} kmol^{-1}$
L	Total height of dispersion	m
g	Standard acceleration of gravity	ms^{-2}
$D_{ m eff,z,G}$	Eff. axial dispersion coefficient, gas	$m^2 s^{-1}$
$D_{ m eff,z,L}$	Eff. axial dispersion coefficient, liquid	$m^2 s^{-1}$
$C_{p,G}$	Spec. heat (at constant pressure), Gas	$Jkg^{-1}K^{-1}$
$C_{p,S}$	Spec. heat (at constant pressure), Solid	$Jkg^{-1}K^{-1}$
$C_{p,L}$	Spec. heat (at constant pressure), Liquid	$Jkg^{-1}K^{-1}$
$C_{p,SL}$	Spec. heat (at constant pressure), Slurry	$Jkg^{-1}K^{-1}$
U	Thermal Transmittance Number	$Wm^{-2}K^{-1}$
d_t	Diameter of tube	m
h_L	Heat transfer coefficient between slurry and gas	$Wm^{-2}K^{-1}$
a	Interfacial area density	$m^2 m^{-3} = m^{-1}$
$\lambda_{ m eff,z,G}$	Eff. thermal conductivity, gas	$Wm^{-1}K^{-1}$
$k_{ m eff,z,L}$	Eff. thermal conductivity, liquid	$Wm^{-1}K^{-1}$
$k_{ m eff,z,S}$	Eff. thermal conductivity, solid	$Wm^{-1}K^{-1}$
$k_{ m eff,z,SL}$	Eff. thermal conductivity, slurry	$Wm^{-1}K^{-1}$
k_G	Thermal conductivity, gas	$Wm^{-1}K^{-1}$
k_L	Thermal conductivity, liquid	$Wm^{-1}K^{-1}$
k_{SL}	Thermal conductivity, slurry	$Wm^{-1}K^{-1}$
μ_G	Viscosity, gas	$Pas = kgs^{-1}m^{-1}$
μ_L	Viscosity, liquid	$Pas = kgs^{-1}m^{-1}$
μ_{SL}	Viscosity, slurry	$Pas = kgs^{-1}m^{-1}$
ΔH_r	Reaction heat	$Jkmol^{-1}$
h_W	Heat transfer coefficient between slurry and wall	$Wm^{-2}K^{-1}$
S_I	Perimeter	m
S_c	Perimeter of column	m
S_t	Perimeter of cooling tube	m
A	Area	m^2
D_c	Diameter of column	m
A_t	Area of cooling tube	m^2
N_t	Number of cooling tubes	_
d_s^*	Sauter mean diameter	m

Table 2: Subscript and Superscript list

symbol	name
*	At the phase boundary
0	Initial (at the inlet)
i	Component number (or name)
s	Superficial
c	Column
t	Cooling tube
p	Constant pressure
w	Column wall
G	Gas Side / Phase
L	Liquid Side / Phase
S	Solid (catalyst) Side / Phase
SL	Slurry Phase (liquid $+$ catalyst)
SK	Catalyst skeleton (material excluding pores)
z	Along the z direction
cat	Catalyst
eff	Effective (sum of molecular and turbulent contributions)

2 Starting point

The general axial dispersion model (ADM) for two-phase flow, with reaction in the liquid (slurry) phase and heat exchange in the liquid (slurry) phase, is taken from Jakobsen (2008) [1], section 8.4, page 767, equations 8.1 to 8.5. Equation 6 (liquid (slurry) phase mass balance), is added.

2.1 Gas Phase Equations

$$\frac{d}{dz}\left(\rho_G v_G^s \omega_{i,G}\right) = \frac{d}{dz}\left(\epsilon_G \rho_G D_{\text{eff,z,G}} \frac{d\omega_{i,G}}{dz}\right) - k_{L,i} a \rho_L(\omega_{L,i}^* - \omega_{L,i}) \tag{1}$$

$$\rho_G C_{p,G} v_G^s \frac{dT_G}{dz} = \frac{d}{dz} \left(\epsilon_G \lambda_{\text{eff},z,G} \frac{dT_G}{dz} \right) - h_L a (T_G - T_{SL})$$
 (2)

$$\frac{d}{dz}\left(\rho_G v_G^s\right) = -\sum_i k_{L,i} a \rho_L (\omega_{L,i}^* - \omega_{L,i}) \tag{3}$$

2.2 Liquid Phase Equations

$$\frac{d}{dz}\left(\rho_L v_L^s \omega_{i,L}\right) = \frac{d}{dz}\left(\epsilon_L \rho_L D_{\text{eff,z,L}} \frac{d\omega_{i,L}}{dz}\right) + k_{L,i} a \rho_L (\omega_{L,i}^* - \omega_{L,i}) + \epsilon_L \sum_r \nu_{i,r} R_{L,r}$$
(4)

$$\rho_L C_{p,L} v_L^s \frac{dT_L}{dz} = \frac{d}{dz} \left(\epsilon_L k_{\text{eff,z,L}} \frac{dT_L}{dz} \right) + 4 \frac{U}{d_t} (T_{\text{sur}} - T_L) + h_L a (T_G - T_L) + \epsilon_L \sum_r (-\Delta H_r) R_{r,L}$$
 (5)

$$\frac{d}{dz}\left(\rho_L v_L^s\right) = \sum_i k_{L,i} a \rho_L (\omega_{L,i}^* - \omega_{L,i}) \tag{6}$$

2.3 Boundary Conditions

Boundary conditions are given in equations 8.6 to 8.9 in Jakobsen (2008) [1].

3 Assumptions

- Perfectly mixed slurry phase consisting of liquid with suspended catalyst particles.
- Constant volume fraction of solids, ϵ_S .
- Only the slurry phase exchanges heat with the wall.
- The pressure is the same in the gas and in the slurry phase; $p_G = p_L$, and follows a hydrostatic profile along the reactor height.
- Ideal gas law valid for gas phase, pV = nRT.
- Reaction takes place in the liquid.
- Neglecting mass transfer resistance in gas film, i.e. $\rho_{G,i}^* \approx \rho_{G,i}$

- Equilibrium at the phase boundary between gas and liquid; $y_i^* = k_i x_i^*$
- $k_{L,i}a(\rho_{L,i}^* \rho_{L,i}) = k_{L,i}a\rho_L(\omega_{i,L}^* \omega_{i,L})$
- Assume mass transfer resistance across liquid film surrounding catalyst pellet, and resistance inside pellet, much less than mass transfer resistance across phase boundary (GL).
- Constant liquid density, $\frac{d\rho_L}{dz} \approx 0$.
- Constant axial dispersion coefficient in both phases, $D_{\rm eff,z,L}$ and $D_{\rm eff,z,G}$.
- Constant liquid velocity $v_L = \frac{v_L^s}{\epsilon_L}$ (but **not** constant superficial velocity v_L^s , i.e. ϵ_L and v_L^s are changing, but v_L is constant).
- Constant thermal conductivity along z direction in both gas and slurry, $\lambda_{\rm eff,z,G}$ and $k_{\rm eff,z,SL}$

4 Kinetic Model

The kinetic model by Yates and Satterfield (1991) [2] is used.

$$r_{CO} = \frac{ap_{\text{CO}}p_{\text{H}_2}}{\left(1 + bp_{\text{CO}}\right)^2} \tag{7}$$

The original units are

$$a[=] \frac{mmol}{min g_{cat} M P a^{2}}$$

$$b[=] \frac{1}{MPa}$$

$$r_{CO}[=] \frac{\frac{mmol}{min g_{cat} M P a^{2}} M P a M P a}{1 + \frac{1}{MPa} M P a} = \frac{mmol}{min g_{cat}}$$

$$(8)$$

Converting to SI units gives

$$a[=] \frac{min}{60s} \frac{mol}{1000mmol} \frac{kmol}{1000mol} \frac{1000g_{cat}}{kg_{cat}} \frac{mmol}{min g_{cat}MPa^2} \frac{MPa^2}{10^610^6Pa^2}$$

$$= \frac{10^3}{60 \cdot 10^3 \cdot 10^3 \cdot 10^6 \cdot 10^6} \frac{kmol}{s \cdot kg_{cat} \cdot Pa^2}$$

$$= \frac{10^{-15}}{60} \frac{kmol}{s \cdot kg_{cat} \cdot Pa^2}$$

$$b[=] \frac{1}{MPa}$$

$$= \frac{1}{MPa} \frac{MPa}{10^6Pa}$$

$$= \frac{10^{-6}}{Pa}$$

$$= \frac{10^{-6}}{Pa}$$

$$r_{CO}[=] \frac{10^{-15}}{60} \frac{kmol}{s \cdot kg_{cat} \cdot Pa^2} \cdot PaPa}{1 + \frac{10^{-6}}{Pa} \cdot Pa}$$

$$(9)$$

Furthermore, it is desired to express the components CO and H₂ in terms of their fractions in the liquid phase. We have from the assumptions that

$$y_i^* = k_i x_i^* \tag{10}$$

and can then write

$$p_i^* = y_i^* p = k_i x_i^* p (11)$$

The final reaction rate expression is thus:

$$r_{CO} = \frac{10^{-15}}{60} \frac{ak_{CO}x_{CO}^*p \, k_{H_2}x_{H_2}^*p}{1 + b \, 10^{-6} \, k_{CO}x_{CO}^*p}$$

$$r_{CO} = \frac{10^{-15}}{60} \frac{ak_{CO}x_{CO}^* \, k_{H_2}x_{H_2}^*p^2}{1 + b \, 10^{-6} \, k_{CO}x_{CO}^*p}$$
(12)

5 Reaction Term

The reaction term from [1] was given as in equation 13.

$$\epsilon_L \sum_r \nu_{i,r} R_{L,r} \tag{13}$$

As the number of reactions in the chosen kinetic model is 1 (Yates and Satterfield (1991)) [2], we can remove the summation sign in 13 to obtain the expression given in 14

$$\epsilon_L \nu_i R_L$$
 (14)

The reaction rate expression R_L taken from [2] and discussed in section 4 was finally obtained in equation 12 in the units $r_{CO}[=]\frac{kmol}{s\,kg_{cat}}$. Studying equations 32 and 33, we see that the reaction term $\frac{\epsilon_L R_i}{\rho_L v_L^s}$ overall shall have the units $\frac{1}{m}$. This requires the units $\epsilon_L R_i[=]\frac{kg\,m}{m^3\,s}\frac{1}{m}$. We see that this requires the following expression for R_i :

$$[\epsilon_L R_i] = \frac{kg \, m}{m^3 \, s} \frac{1}{m} = [X][\epsilon_L \nu_i r_{CO}] = [X] \frac{kmol}{s \, kg_{cat}}$$

$$[X] = \frac{[\epsilon_L R_i]}{[\epsilon_L \nu_i r_{CO}]} = \frac{\frac{kg \, m}{m^3 \, s} \frac{1}{m}}{\frac{kmol}{s \, kg_{cat}}} = \frac{kg}{kmol} \frac{kg_{cat}}{m^3} = [M_{w,i}][\rho_{cat}]$$

$$(15)$$

The final reaction rate term to be inserted into equation 33 is thus

$$\frac{\epsilon_L \nu_i r_{CO}}{\rho_L v_L^s} M_{w,i} \rho_{cat} \tag{16}$$

6 Mass Transfer Term

We have

$$k_{L,i}a\rho_L(\omega_{i,L}^* - \omega_{i,L}) \tag{17}$$

The equilibrium criterium at the phase boundary between gas and liquid is given in equation 18.

$$y_i^* = k_i x_i^* \tag{18}$$

The mole fraction x_i can be expressed in terms of mass fraction ω_i as given in equation 19.

$$x_i = \frac{\frac{\omega_i}{M_{w,i}}}{\sum_j \left(\frac{\omega_j}{M_{w,j}}\right)} \tag{19}$$

Inserting for y_i^* and x_i^* in equation 18 gives

$$\frac{\frac{\omega_{i,G}^*}{M_{w,i}}}{\sum_{j} \left(\frac{\omega_{j,G}^*}{M_{w,j}}\right)} = k_i \frac{\frac{\omega_{i,L}^*}{M_{w,i}}}{\sum_{j} \left(\frac{\omega_{j,L}^*}{M_{w,j}}\right)}$$
(20)

Recognising the definition for average molar mass (equation 21) in terms of mass fractions, we can write the equilibrium expression as in equation 22.

$$\overline{M_w} = \sum_{i} x_i M_{w,i} = \sum_{i} M_{w,i} \frac{\frac{\omega_i}{M_{w,i}}}{\sum_{j} \left(\frac{\omega_j}{M_{w,j}}\right)} = \sum_{i} \frac{\omega_i}{\sum_{j} \left(\frac{\omega_j}{M_{w,j}}\right)} = \frac{1}{\sum_{j} \left(\frac{\omega_j}{M_{w,j}}\right)}$$
(21)

$$\frac{\omega_{i,G}^*}{\sum_{j} \left(\frac{\omega_{j,G}^*}{M_{w,j}}\right)} = k_i \frac{\omega_{i,L}^*}{\sum_{j} \left(\frac{\omega_{j,L}^*}{M_{w,j}}\right)}$$

$$\overline{M_G} \omega_{i,G}^* = k_i \overline{M_L} \omega_{i,L}^*$$
...
$$\omega_{i,L}^* = \frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^*$$
(22)

The final form of the mass transfer terms is given in equation 23.

$$k_{L,i}a\rho_L(\frac{1}{k_i}\frac{\overline{M_G}}{\overline{M_L}}\omega_{i,G}^* - \omega_{i,L})$$
(23)

7 Heat Transfer Terms

7.1 Heat transfer between slurry and gas

The heat transfer between slurry and gas is given by

$$h_L a (T_G - T_{SL}) \tag{24}$$

7.2 Heat transfer between slurry and wall (cooling)

The reaction is exothermal. Heat is removed by cooling tubes inside the reactor.

The heat transfer term denoting the cooling of the slurry by cooling tubes, $\frac{4U}{d_t}(T_{\text{sur}} - T_{SL})$, must be re-written. The starting point from Jakobsen (2008) [1], section 8.4, page 767 considers heating on the outside of the reactor perimeter only, but for Fischer-Tropsch synthesis an arrangment of multiple coolant tubes inside the reactor is more common. A more general form of the heat transfer term by cooling is given in Jakobsen (2008) [1], equation 1.291:

$$-h_W \frac{S_I}{A} (\langle T \rangle_A - \langle T \rangle_W) \tag{25}$$

Considering a cooling arrangement with N_t coolant tubes with the same length as the dispersion having a constant cross-sectional area A_t , we can write the perimeter S_I and area A of the cooling surface at each level of z as:

$$S_{I} = 2\pi \frac{D_{c}}{2} + N_{t}S_{t} = \pi D_{c} + N_{t}\pi d_{t} = \pi \left(D_{c} + N_{t}d_{t}\right)$$

$$A = A_{\text{column}} - A_{\text{coolingtubes}} = \pi \left(\frac{D_{c}}{2}\right)^{2} - N_{t}A_{t} = \frac{\pi}{4}D_{c}^{2} - N_{t}\frac{\pi}{4}d_{t}^{2} = \frac{\pi}{4}\left(D_{c}^{2} - N_{t}d_{t}^{2}\right)$$
(26)

This gives for the heat transfer term due to cooling of slurry:

$$-h_W \frac{S_I}{A} (\langle T \rangle_A - \langle T \rangle_W) = h_W \frac{\pi (D_c + N_t d_t)}{\frac{\pi}{4} (D_c^2 - N_t d_t^2)} (T_{\text{surr}} - T_{SL}) = h_W \frac{D_c + N_t d_t}{\frac{1}{4} (D_c^2 - N_t d_t^2)} (T_{\text{surr}} - T_{SL})$$
(27)

8 Mass and Species Mass Conservation equations

8.1 Total mass conservation: gas phase

For the total mass balance for the gas phase, equation 3, the left hand side is expanded and the equation is manipulated to obtain an expression for the change in superficial gas velcocity by reactor length $\frac{d}{dz}v_G^s$ alone on the left hand side.

$$\frac{d}{dz}(\rho_G v_G^s) = -\rho_L \sum_i k_{L,i} a(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L})$$

$$\rho_G \frac{d}{dz} v_G^s + v_G^s \frac{d}{dz} \rho_G = -\rho_L \sum_i k_{L,i} a(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L})$$

$$\frac{d}{dz} v_G^s = -\frac{v_G^s}{\rho_G} \frac{d}{dz} \rho_G - \frac{\rho_L}{\rho_G} \sum_i k_{L,i} a(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L})$$
(28)

8.2 Species mass conservation: gas phase

Utilising the assumptions made in section 3, the gas phase component balance on mass basis is given in equation 30, upper part. The left hand side term is then expanded (equation 30, middle part), along with the dispersion term (accepting constant dispersion coefficient), and finally the equation is manipulated to obtain the partial derivative of the mass fraction $\frac{d}{dz}\omega_{i,G}$ terms at the

left hand side (equation 30).

$$\frac{d}{dz}\left(\rho_{G}v_{G}^{s}\omega_{i,G}\right) = \frac{d}{dz}\left(\epsilon_{G}\rho_{G}D_{\text{eff,z,G}}\frac{d\omega_{i,G}}{dz}\right) - k_{L,i}a\rho_{L}\left(\frac{1}{k_{i}}\frac{\overline{M_{G}}}{\overline{M_{L}}}\omega_{i,G}^{*} - \omega_{i,L}\right)$$

$$\rho_{G}v_{G}^{s}\frac{d}{dz}\omega_{i,G} + \rho_{G}\omega_{i,G}\frac{d}{dz}v_{G}^{s} + v_{G}^{s}\omega_{i,G}\frac{d}{dz}\rho_{G} = \rho_{G}D_{\text{eff,z,G}}\frac{d\omega_{i,G}}{dz}\frac{d\epsilon_{G}}{dz} + \epsilon_{G}\rho_{G}\frac{d\omega_{i,G}}{dz}\frac{dD_{\text{eff,z,G}}}{dz}$$

$$+ \epsilon_{G}D_{\text{eff,z,G}}\frac{d\omega_{i,G}}{dz}\frac{d\rho_{G}}{dz} + \epsilon_{G}\rho_{G}D_{\text{eff,z,G}}\frac{d^{2}\omega_{i,G}}{dz^{2}} - k_{L,i}a\rho_{L}\left(\frac{1}{k_{i}}\frac{\overline{M_{G}}}{\overline{M_{L}}}\omega_{i,G}^{*} - \omega_{i,L}\right)$$

$$\left[\rho_{G}v_{G}^{s} - \rho_{G}D_{\text{eff,z,G}}\frac{d\epsilon_{G}}{dz} - \epsilon_{G}D_{\text{eff,z,G}}\frac{d\rho_{G}}{dz}\right]\frac{d\omega_{i,G}}{dz} + \left[-\epsilon_{G}\rho_{G}D_{\text{eff,z,G}}\right]\frac{d^{2}\omega_{i,G}}{dz^{2}} =$$

$$- \rho_{G}\omega_{i,G}\frac{dv_{G}^{s}}{dz} - v_{G}^{s}\omega_{i,G}\frac{d\rho_{G}}{dz} - k_{L,i}a\rho_{L}\left(\frac{1}{k_{i}}\frac{\overline{M_{G}}}{\overline{M_{L}}}\omega_{i,G}^{*} - \omega_{i,L}\right)$$
(29)

Dividing by $\rho_G v_G^s$ and inserting for $\frac{dv_G^s}{dz}$ (equation 28) gives:

$$\begin{split} &\left[1 - \frac{D_{\mathrm{eff,z,G}}}{v_G^s} \frac{d\epsilon_G}{dz} - \frac{1}{\rho_G v_G^s} \frac{d\rho_G}{dz}\right] \frac{d\omega_{i,G}}{dz} - \epsilon_G \frac{D_{\mathrm{eff,z,G}}}{v_G^s} \frac{d^2\omega_{i,G}}{dz^2} = \\ &\frac{\omega_{i,G}}{\rho_G} \frac{d\rho_G}{dz} + \frac{\omega_{i,G}}{v_G^s} \frac{\rho_L}{\rho_G} \sum_i k_{L,i} a (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) - \frac{\omega_{i,G}}{\rho_G} \frac{d\rho_G}{dz} - \frac{\rho_L}{\rho_G} \frac{k_{L,i} a}{v_G^s} (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) \\ &\left[1 - \frac{D_{\mathrm{eff,z,G}}}{v_G^s} \frac{d\epsilon_G}{dz} - \frac{1}{\rho_G v_G^s} \frac{d\rho_G}{dz}\right] \frac{d\omega_{i,G}}{dz} - \epsilon_G \frac{D_{\mathrm{eff,z,G}}}{v_G^s} \frac{d^2\omega_{i,G}}{dz^2} = \\ &\frac{\omega_{i,G}}{v_G^s} \frac{\rho_L}{\rho_G} \sum_i k_{L,i} a (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) - \frac{\rho_L}{\rho_G} \frac{k_{L,i} a}{v_G^s} (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) \end{split}$$

(30)

8.3 Total mass conservation: liquid phase

For the total mass balance in the liquid phase, we insert for the mass transfer term (equation 23) into equation 6. Further, we expand the left hand side and obtain an expression for $\frac{d}{dz}v_L^s$.

$$\frac{d}{dz}\left(\rho_L v_L^s\right) = \rho_L \sum_i k_{L,i} a\left(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}\right)$$

$$\rho_L \frac{d}{dz} v_L^s + v_L^s \frac{d}{dz} \rho_L = \rho_L \sum_i k_{L,i} a\left(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}\right)$$

$$\frac{d}{dz} v_L^s = -\frac{v_L^s}{\rho_L} \frac{d}{dz} \rho_L + \sum_i k_{L,i} a\left(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}\right)$$
(31)

8.4 Species mass conservation: liquid phase

Similar manipulations as performed to the gas phase equations in subsection 8.2 are performed to the liquid phase equations, see equations 32 and 31.

$$\frac{d}{dz}\left(\rho_{L}v_{L}^{s}\omega_{i,L}\right) = \frac{d}{dz}\left(\epsilon_{L}\rho_{L}D_{\text{eff,z,L}}\frac{d\omega_{i,L}}{dz}\right) + k_{L,i}a\rho_{L}\left(\frac{1}{k_{i}}\frac{\overline{M_{L}}}{\overline{M_{G}}}\omega_{i,G}^{*} - \omega_{i,L}\right) + \epsilon_{L}R_{i}$$

$$\rho_{L}v_{L}^{s}\frac{d}{dz}\omega_{i,L} + \rho_{L}\omega_{i,L}\frac{d}{dz}v_{L}^{s} + v_{L}^{s}\omega_{i,L}\frac{d}{dz}\rho_{L} = \frac{d}{dz}\left(\epsilon_{L}\rho_{L}D_{\text{eff,z,L}}\frac{d\omega_{i,L}}{dz}\right) + k_{L,i}a\rho_{L}\left(\frac{1}{k_{i}}\frac{\overline{M_{G}}}{\overline{M_{L}}}\omega_{i,G}^{*} - \omega_{i,L}\right) + \epsilon_{L}R_{i}$$

$$\frac{d}{dz}\omega_{i,L} = -\frac{\omega_{i,L}}{v_{L}^{s}}\frac{d}{dz}v_{L}^{s} - \frac{\omega_{i,L}}{\rho_{L}}\frac{d}{dz}\rho_{L} + \frac{1}{\rho_{L}v_{L}^{s}}\frac{d}{dz}\left(\epsilon_{L}\rho_{L}D_{\text{eff,z,L}}\frac{d\omega_{i,L}}{dz}\right) + \frac{k_{L,i}a}{v_{L}^{s}}\left(\frac{1}{k_{i}}\frac{\overline{M_{G}}}{\overline{M_{L}}}\omega_{i,G}^{*} - \omega_{i,L}\right) + \frac{\epsilon_{L}R_{i}}{\rho_{L}v_{L}^{s}}$$

$$\frac{d}{dz}\omega_{i,L} = -\frac{\omega_{i,L}}{v_{L}^{s}}\frac{d}{dz}v_{L}^{s} - \frac{\omega_{i,L}}{\rho_{L}}\frac{d}{dz}\rho_{L} + \frac{1}{\rho_{L}v_{L}^{s}}\frac{d}{dz}\left(\epsilon_{L}\rho_{L}D_{\text{eff,z,L}}\frac{d\omega_{i,L}}{dz}\right) + \frac{k_{L,i}a}{v_{L}^{s}}\left(\frac{1}{k_{i}}\frac{\overline{M_{G}}}{\overline{M_{L}}}\omega_{i,G}^{*} - \omega_{i,L}\right) + \frac{\epsilon_{L}R_{i}}{\rho_{L}v_{L}^{s}}$$

$$\frac{d}{dz}\omega_{i,L} = -\frac{\omega_{i,L}}{v_{L}^{s}}\frac{d}{dz}v_{L}^{s} - \frac{\omega_{i,L}}{\rho_{L}}\frac{d}{dz}\rho_{L} + \frac{1}{\rho_{L}v_{L}^{s}}\frac{d}{dz}\left(\epsilon_{L}\rho_{L}D_{\text{eff,z,L}}\frac{d\omega_{i,L}}{dz}\right) + \frac{k_{L,i}a}{v_{L}^{s}}\left(\frac{1}{k_{i}}\frac{\overline{M_{G}}}{\overline{M_{L}}}\omega_{i,G}^{*} - \omega_{i,L}\right) + \frac{\epsilon_{L}R_{i}}{\rho_{L}v_{L}^{s}}$$

$$\frac{d}{dz}\omega_{i,L} = -\frac{\omega_{i,L}}{v_{L}^{s}}\frac{d}{dz}v_{L}^{s} - \frac{\omega_{i,L}}{\rho_{L}}\frac{d}{dz}\rho_{L} + \frac{1}{\rho_{L}v_{L}^{s}}\frac{d}{dz}\left(\epsilon_{L}\rho_{L}D_{\text{eff,z,L}}\frac{d\omega_{i,L}}{dz}\right) + \frac{k_{L,i}a}{v_{L}^{s}}\left(\frac{1}{k_{L}}\frac{\overline{M_{G}}}{\overline{M_{G}}}\right)$$

$$\frac{d}{dz}\omega_{i,L} = -\frac{\omega_{i,L}}{v_{L}^{s}}\frac{d}{dz}v_{L}^{s} - \frac{\omega_{i,L}}{\rho_{L}}\frac{d}{dz}\rho_{L} + \frac{1}{\rho_{L}v_{L}^{s}}\frac{d}{dz}\left(\epsilon_{L}\rho_{L}D_{\text{eff,z,L}}\frac{d\omega_{i,L}}{dz}\right) + \frac{k_{L,i}a}{v_{L}^{s}}\frac{d\omega_{i,L}}{\overline{M_{G}}} + \frac{k_{L,i}a}{v$$

Inserting for equation 31 into equation 32 gives equation 33. The axial dispersion term is ex-

panded.

$$\begin{split} \frac{d}{dz}\omega_{i,L} &= -\frac{\omega_{i,L}}{v_L^s} \left[-\frac{v_L^s}{\rho_L} \frac{d}{dz} \rho_L + \sum_i k_{L,i} a (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) \right] \\ &- \frac{\omega_{i,L}}{\rho_L} \frac{d}{dz} \rho_L + \frac{1}{\rho_L v_L^s} \frac{d}{dz} \left(\epsilon_L \rho_L D_{\text{eff},z,L}} \frac{d\omega_{i,L}}{dz} \right) + \frac{k_{L,i} a}{v_L^s} (\frac{1}{k_i} \frac{\overline{M_L}}{\overline{M_G}} \omega_{i,G}^* - \omega_{i,L}) + \frac{\epsilon_L R_i}{v_L^s \rho_L} \\ \frac{d}{dz}\omega_{i,L} &= \frac{\omega_{i,L}}{v_L^s} \frac{v_L^s}{\rho_L} \frac{d}{dz} \rho_L - \frac{\omega_{i,L}}{v_L^s} \sum_i k_{L,i} a (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) \\ &- \frac{\omega_{i,L}}{\rho_L} \frac{d}{dz} \rho_L + \frac{1}{\rho_L v_L^s} \frac{d}{dz} \left(\epsilon_L \rho_L D_{\text{eff},z,L}} \frac{d\omega_{i,L}}{dz} \right) + \frac{k_{L,i} a}{v_L^s} (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) + \frac{\epsilon_L R_i}{\rho_L v_L^s} \\ \frac{d}{dz}\omega_{i,L} &= -\frac{\omega_{i,L}}{v_L^s} \sum_i k_{L,i} a (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) + \frac{1}{\rho_L v_L^s} \frac{d}{dz} \left(\epsilon_L \rho_L D_{\text{eff},z,L}} \frac{d\omega_{i,L}}{dz} \right) \\ &+ \frac{k_{L,i} a}{v_L^s} (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) + \frac{\epsilon_L R_i}{v_L^s \rho_L} \\ \frac{d}{dz}\omega_{i,L} &= -\frac{\omega_{i,L}}{v_L^s} \sum_i k_{L,i} a (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) \\ &+ \frac{\rho_L D_{\text{eff},z,L}}{\rho_L v_L^s} \frac{d\epsilon_L}{dz} + \frac{\epsilon_L D_{\text{eff},z,L}}{\rho_L v_L^s} \frac{d\omega_{i,L}}{dz} \frac{d\rho_L}{dz} + \frac{\epsilon_L \rho_L}{\rho_L v_L^s} \frac{d\omega_{i,L}}{dz} \frac{d\rho_L}{dz} + \frac{\epsilon_L \rho_L}{\rho_L v_L^s} \frac{d\omega_{i,L}}{dz} \frac{d\rho_L}{dz} + \frac{\epsilon_L \rho_L}{\rho_L v_L^s} \frac{d\omega_{i,L}}{dz} \frac{d^2\omega_{i,L}}{dz^2} \\ &+ \frac{k_{L,i} a}{v_L^s} (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) + \frac{\epsilon_L R_i}{v_L^s} \frac{d\omega_{i,L}}{dz} \frac{d\epsilon_L}{dz} + \frac{\epsilon_L D_{\text{eff},z,L}}{v_L^s} \frac{d^2\omega_{i,L}}{dz^2} \\ &+ \frac{k_{L,i} a}{v_L^s} (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) + \frac{\epsilon_L R_i}{v_L^s} \frac{d\omega_{i,L}}{dz} \frac{d\epsilon_L}{dz} + \frac{\epsilon_L D_{\text{eff},z,L}}{dz} \frac{d^2\omega_{i,L}}{dz^2} \\ &+ \frac{k_{L,i} a}{v_L^s} (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) + \frac{\epsilon_L R_i}{v_L^s} \frac{d^2\omega_{i,L}}{dz^2} \\ &= -\frac{\omega_{i,L}}{v_L^s} \sum_i k_{L,i} a (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) + \frac{k_{L,i} a}{v_L^s} (\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}) + \frac{\epsilon_L R_i}{v_L^s} \frac{d^2\omega_{i,L}}{dz^2} \\ &= -\frac{\omega_{i,L}}{v_L^s} \sum_i k_{$$

8.5 Rate of Change in Volume Fraction

Equation 33 requires an expression for the rate of change in volume fraction of liquid, $\frac{d\epsilon_L}{dz}$. An expression for this can be found using the continuity equation for the liquid phase, equation 31,

by replacing the superficial velocity with its definition $v_L^s = \epsilon_L v_L$. This gives:

$$\frac{d}{dz}(\rho_L v_L^s) = \rho_L \sum_i k_{L,i} a(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L})$$

$$\frac{d}{dz}(\rho_L \epsilon_L v_L) = \rho_L \sum_i k_{L,i} a(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L})$$

$$\epsilon_L v_L \frac{d\rho_L}{dz} + \rho_L v_L \frac{d\epsilon_L}{dz} + \rho_L \epsilon_L \frac{dv_L}{dz} = \rho_L \sum_i k_{L,i} a(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L})$$

$$\frac{d\epsilon_L}{dz} = \frac{1}{v_L} \sum_i k_{L,i} a(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L})$$

$$\frac{d\epsilon_L}{dz} = \frac{\epsilon_L}{v_L^s} \sum_i k_{L,i} a(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L})$$
(34)

where the assumptions of $\frac{d\rho_L}{dz} = 0$ and $\frac{dv_L}{dz} = 0$ are utilised.

8.6 Rate of Change in Density

Equations 30 and 28 require an expression for the rate of change in gas density, $\frac{d}{dz}\rho_G$.

The ideal gas law (35) was assumed to be valid in section 3. An expression for gas density given the ideal gas law valid is given in

$$pV = nRT (35)$$

$$\rho_G = \frac{n}{V}\overline{M_G} = \frac{p\overline{M_G}}{RT} \tag{36}$$

This yields the expression shown in equation 37.

$$\frac{d}{dz}\rho_G = \frac{d}{dz}\left(\frac{p\overline{M_G}}{RT}\right) = \frac{p}{RT}\frac{d}{dz}\overline{M_G} + \frac{\overline{M_G}}{RT}\frac{dp}{dz} - \frac{p\overline{M_G}}{R}\frac{dT_G}{dz}$$
(37)

Equation 37 requires an expression for the rate of change in average molar mass for the gas phase $\frac{d}{dz}\overline{M_G}$ and for the pressure $\frac{dp}{dz}$. These are derived in sections 8.8 and 8.7, respectively.

8.7 Rate of Change in Pressure

A hydrostatic pressure profile is applied;

$$p(z) = \int_0^L \rho_{\text{tot}}(z)gdz \tag{38}$$

The total density $\rho_{\rm tot}$ is assumed constant and given by

$$\rho_{\text{tot}} = \epsilon_G^0 \rho_G^0 + \epsilon_L^0 \rho_L + \epsilon_s \rho_s \tag{39}$$

Inserting for $\rho_{\rm tot}(z) = \rho_{\rm tot}$ and utilising h = L - z

$$p(z) = \int_0^h \rho_{\text{tot}} g dz$$

$$p(z) = \rho_{\text{tot}} g h$$

$$p(z) = \rho_{\text{tot}} g (L - z)$$

$$(40)$$

Differentiating with respect to z then gives

$$\frac{dp}{dz} = -\rho_{\text{tot}}g\tag{41}$$

8.8 Rate of Change in Average Molar Mass

Equation 21 provides us with an expression for $\overline{M_G}$, which we insert into equation 37 and differentiate. The result is given below.

$$\frac{d}{dz}\overline{M_G} = \frac{d}{dz}\left(\sum_{i}x_{i}M_{w,i}\right) = \sum_{i}M_{w,i}\frac{d}{dz}\left(\frac{\omega_{i}^G}{M_{w,i}}\right) \\
= \sum_{i}M_{w,i}\left[\frac{\omega_{i}^G}{M_{w,i}}\frac{d}{dz}\left(\frac{1}{\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}}\right) + \frac{1}{\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}}\frac{1}{M_{w,i}}\frac{d\omega_{i}^G}{dz}\right] \\
= \sum_{i}\left[\omega_{i}^G\frac{d}{dz}\left(\frac{1}{\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}}\right) + \frac{1}{\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}}\frac{d\omega_{i}^G}{dz}\right] \\
= \sum_{i}\left[\omega_{i}^G\left(-\frac{1}{\left(\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}\right)^2}\sum_{i}\left[\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}\frac{d\omega_{j}^G}{dz}\right]\right) + \frac{1}{\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}}\frac{d\omega_{i}^G}{dz}\right] \\
= \sum_{i}\left[\omega_{i}^G\left(-\frac{1}{\left(\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}\right)^2}\left[\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}\frac{d\omega_{j}^G}{dz}\right]\right) + \frac{1}{\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}}\frac{d\omega_{i}^G}{dz}\right] \\
= \sum_{i}\left[\frac{1}{\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}}\frac{d\omega_{i}^G}{dz} - \omega_{i}^G\frac{\sum_{j}\frac{1}{M_{w,j}}\frac{d\omega_{j}^G}{dz}}{\left(\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}\right)^2}\right] \\
= \sum_{i}\left[\frac{\frac{d\omega_{i}^G}{dz}\sum_{j}\frac{\omega_{j}^G}{M_{w,j}} - \omega_{i}^G\sum_{j}\frac{1}{M_{w,j}}\frac{d\omega_{j}^G}{dz}}{\left(\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}\right)^2}\right] \\
= \sum_{i}\left[\frac{\frac{d\omega_{i}^G}{dz}\sum_{j}\frac{\omega_{j}^G}{M_{w,j}} - \omega_{i}^G\sum_{j}\frac{d\omega_{j}^G}{M_{w,j}}}{\left(\sum_{j}\frac{\omega_{j}^G}{M_{w,j}}\right)^2}\right] \\
= \frac{d}{dz}\overline{M_G} = \frac{1}{\left(\sum_{i}\frac{\omega_{j}^G}{M_{w,j}}\right)^2}\sum_{i}\left[\frac{d\omega_{i}^G}{dz}\sum_{j}\frac{\omega_{j}^G}{M_{w,j}} - \omega_{i}^G\sum_{j}\frac{d\omega_{j}^G}{M_{w,j}}\right] \\$$

9 Energy Conservation

The starting point for the temperature equations was given in equations 2 and 5. As stated in the section of Assumptions, 3, the thermal conductivity coefficient is constant for both phases.

9.1 Temperature equation: gas phase

$$\rho_G C_{p,G} v_G^s \frac{dT_G}{dz} = \frac{d}{dz} \left(\epsilon_G \lambda_{\text{eff},z,G} \frac{dT_G}{dz} \right) - h_L a (T_G - T_{SL})$$
(43)

Expanding the conductivity term and collecting all $\frac{dT_G}{dz}$ terms on the left hand side gives:

$$\left[\rho_G C_{p,G} v_G^s - \lambda_{\text{eff,z,G}} \frac{d\epsilon_G}{dz}\right] \frac{dT_G}{dz} - \epsilon_G \lambda_{\text{eff,z,G}} \frac{d^2 T_G}{dz^2} = -h_L a (T_G - T_{SL})$$
(44)

9.2 Temperature equation: slurry phase

$$\rho_{SL}C_{p,SL}v_{SL}^{s}\frac{dT_{SL}}{dz} = \frac{d}{dz}\left(\epsilon_{SL}k_{\text{eff},z,L}\frac{dT_{SL}}{dz}\right) + h_{W}\frac{S_{I}}{A}(T_{\text{surr}} - T_{SL}) + h_{L}a(T_{G} - T_{SL}) + \epsilon_{SL}\sum_{r}(-\Delta H_{r})r_{CO}\rho_{\text{cat}}$$
(45)

Expanding the conductivity term, accepting constant $k_{\text{eff,z,L}}$ and collecting all $\frac{dT_{SL}}{dz}$ terms on the left hand side gives:

$$\left[\rho_{SL}C_{p,SL}v_{SL}^{s} - k_{\text{eff,z,L}}\frac{d\epsilon_{SL}}{dz}\right]\frac{dT_{SL}}{dz} - \epsilon_{SL}k_{\text{eff,z,L}}\frac{d^{2}T_{SL}}{dz^{2}} = h_{W}\frac{S_{I}}{A}(T_{\text{surr}} - T_{SL}) + h_{L}a(T_{G} - T_{SL}) + \epsilon_{SL}\sum_{r}(-\Delta H_{r})r_{CO}\rho_{\text{cat}}$$

$$(46)$$

10 Parameters

See separate note on the non-adjustable operating conditions.

11 Final Model Equations

$$\epsilon_L + \epsilon_G + \epsilon_S = 1 \tag{47}$$

$$\frac{d\epsilon_L}{dz} = \frac{\epsilon_L}{v_L^s} \sum_i k_{L,i} a \left(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L} \right)
\frac{d\epsilon_S}{dz} = 0
\frac{d\epsilon_G}{dz} = \frac{d(1 - \epsilon_S - \epsilon_L)}{dz} = -\frac{d\epsilon_L}{dz} - \frac{d\epsilon_S}{dz} = -\frac{d\epsilon_L}{dz}$$
(48)

$$\frac{d\rho_G}{dz} = \frac{p}{RT} \frac{d\overline{M}_G}{dz} + \frac{\overline{M}_G}{RT} \frac{dp}{dz} - \frac{\overline{M}_G p \frac{dT_G}{dz}}{RT_G^2}
\frac{d\rho_L}{dz} = 0$$
(49)

$$\frac{d\overline{M_G}}{dz} = \frac{1}{\left(\sum_j \frac{\omega_j^G}{M_{w,j}}\right)^2} \sum_i \left[\frac{d\omega_{G,i}}{dz} \sum_j \frac{\omega_j^G}{M_{w,j}} - \omega_{i,G} \sum_j \frac{d\omega_{G,j}}{dz} \frac{1}{M_{w,j}} \right]
\frac{d\overline{M_L}}{dz} = \frac{1}{\left(\sum_j \frac{\omega_j^L}{M_{w,j}}\right)^2} \sum_i \left[\frac{d\omega_{L,i}}{dz} \sum_j \frac{\omega_j^L}{M_{w,j}} - \omega_{i,L} \sum_j \frac{d\omega_{L,j}}{dz} \frac{1}{M_{w,j}} \right]$$
(50)

$$\frac{d}{dz}v_G^s = -\frac{v_G^s}{\rho_G}\frac{d}{dz}\rho_G - \frac{\rho_L}{\rho_G}\sum_i k_{L,i}a(\frac{1}{k_i}\frac{\overline{M_G}}{\overline{M_L}}\omega_{i,G}^* - \omega_{i,L}^*)$$

$$\frac{d}{dz}v_L^s = -\frac{v_L^s}{\rho_L}\frac{d}{dz}\rho_L + \sum_i k_{L,i}a(\frac{1}{k_i}\frac{\overline{M_G}}{\overline{M_L}}\omega_{i,G}^* - \omega_{i,L}^*)$$
(51)

$$\left[1 - \frac{D_{\text{eff,z,G}}}{v_G^s} \frac{d\epsilon_G}{dz} - \frac{1}{\rho_G v_G^s} \frac{d\rho_G}{dz}\right] \frac{d\omega_{i,G}}{dz} - \epsilon_G \frac{D_{\text{eff,z,G}}}{v_G^s} \frac{d^2\omega_{i,G}}{dz^2}
= \frac{\omega_{i,G}}{v_G^s} \frac{\rho_L}{\rho_G} \sum_i k_{L,i} a \left(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}\right) - \frac{\rho_L}{\rho_G} \frac{k_{L,i}a}{v_G^s} \left(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}\right)
\left[1 - \frac{D_{\text{eff,z,L}}}{v_L^s} \frac{d\epsilon_L}{dz}\right] \frac{d\omega_{i,L}}{dz} - \frac{\epsilon_L D_{\text{eff,z,L}}}{v_L^s} \frac{d^2\omega_{i,L}}{dz^2}
= -\frac{\omega_{i,L}}{v_L^s} \sum_i k_{L,i} a \left(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}\right) + \frac{k_{L,i}a}{v_L^s} \left(\frac{1}{k_i} \frac{\overline{M_G}}{\overline{M_L}} \omega_{i,G}^* - \omega_{i,L}\right) + \frac{\epsilon_L \nu_i r_{CO}}{\rho_L v_L^s} M_{w,i} \rho_{cat}$$
(52)

Energy balance: heat flux and temperature equations Gas phase:

$$\frac{q_G}{\epsilon_G \lambda_{\text{eff,z,G}}} + \frac{dT_G}{dz} = 0$$

$$\frac{dT_G}{dz} + \frac{1}{\rho_G C_{p,G} v_G^s} \frac{dq_G}{dz} + \frac{h_L a}{\rho_G C_{p,G} v_G^s} (T_G - T_{SL}) = 0$$
(53)

Liquid phase:

$$\frac{q_{SL}}{\epsilon_{SL}\lambda_{\text{eff,z,SL}}} + \frac{dT_{SL}}{dz} = 0$$

$$\frac{dT_{SL}}{dz} + \frac{1}{\rho_{SL}C_{p,SL}v_{SL}^{s}} \frac{dq_{SL}}{dz} - h_{W} \frac{S_{I}}{A} \frac{(T_{\text{surr}} - T_{SL})}{\rho_{SL}C_{p,SL}v_{SL}^{s}} - \frac{h_{L}a(T_{G} - T_{SL})}{\rho_{SL}C_{p,SL}v_{SL}^{s}} = \frac{\epsilon_{L} \sum_{r} (-\Delta H_{r})r_{CO}\rho_{\text{cat}}}{\rho_{SL}C_{p,SL}v_{SL}^{s}}$$
(54)

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