Discretized Version for Thesis

Conditions for Problem as found in paper (1226) for pseudo homogenous Model

Initial Conditions for t=0	**Boundary Condition (BC)**
$w_j = w_{j,in}$	$u_z = u_{z,in}$ for z = 0
$T = T_{in}$	Heat flux, $Q_z = 0$ for z=L
$\rho_g = {\rho_g}_{in}$	Diffusion flux, $J_J = 0$ for z=L
	$P = P_{,in}$ for z=0

Uz

Cell centre values

Wj, T,P, ρ_g,P

The general form of the continuity equation is

$\mathcal{E}_b \frac{d\rho_g}{dt} + \frac{\partial}{\partial Z} u_z \rho_g = 0$ …………from equation(9) to get pressure variation

$$\frac{\partial \mathcal{E}_b \rho_g}{dt} = \mathcal{E}_b \frac{\partial \rho_g}{\partial t} + \rho_g \frac{\partial \mathcal{E}_b}{\partial t}$$

$$\mathcal{E}_b \frac{\partial \rho_g}{\partial t} + \rho_g \frac{\partial \mathcal{E}_b}{\partial t} + \frac{\partial}{\partial Z} u_z \rho_g = 0$$

$$\frac{\partial \mathcal{E}_b \rho_g}{dt} = \mathcal{E}_b \frac{\partial \frac{P}{RT}}{\partial t} + \frac{P}{RT} \frac{\partial \mathcal{E}_b}{dP} \frac{\partial P}{\partial t}$$

$$\mathcal{E}_b \frac{\partial \frac{P}{RT}}{\partial t} = f = f(P,T)$$

$$\frac{df}{dt} = \frac{\mathcal{E}_b}{R} \frac{1}{T} \frac{\partial P}{\partial t} + \frac{\mathcal{E}_b}{R} \frac{-P}{T^2} \frac{\partial T}{\partial t}$$

$$\frac{df}{dt} = \frac{P}{RT} \left[\left(\frac{\mathcal{E}_b}{P} \right) \frac{\partial P}{\partial t} - \left(\frac{\mathcal{E}_b}{T} \right) \frac{\partial T}{\partial t} \right]$$

The continuity becomes

$\mathcal{E}_b \rho \left(\frac{1}{P} \right) \frac{\partial P}{\partial t} - \mathcal{E}_b \rho \left(\frac{1}{T} \right) \frac{\partial T}{\partial t} + u_z \rho \frac{\partial P}{\partial z} = 0$………………………..(4.1)

From equation (11)

$\frac{\partial P}{\partial z} = k_D u_z + k_v u_z{}^2$ ……………………….(11)

Equation 11 becomes

$$\frac{\partial P}{\partial z} = -u_z(k_D + k_v u_z)$$

$u_z = \frac{1}{(k_D + k_v u_z)} \frac{\partial P}{\partial z}$…………………………….(11.1)

Introducing a constant , $K_p = \frac{1}{(k_D + k_v u_z)}$ ……………(11.2)

$u_z = -K_p \frac{\partial P}{\partial z}$ …………………………………(11.3)

Substituting equation 11.3 into equation 4.1 yields

$\mathcal{E}_b \rho \left(\frac{1}{P}\right) \frac{\partial P}{\partial t} - \mathcal{E}_b \rho \left(\frac{1}{T}\right) \frac{\partial T}{\partial t} - \frac{\partial}{\partial z} K_p \rho \frac{\partial P}{\partial z} = 0$………………………..(4.1)

The final form of the continuity equation before discretizing gives

$$\mathcal{E}_b \rho \left(\frac{1}{P}\right) \frac{\partial P}{\partial t} - \mathcal{E}_b \rho \left(\frac{1}{T}\right) \frac{\partial T}{\partial t} - \frac{\partial}{\partial z} \rho K_p \frac{\partial P}{\partial z} = 0$$

Discretizing the above yields

$$\left(\frac{\mathcal{E}_{b}{}_i^k \times \rho_i^k}{P_i^k \times \Delta t}\right)\left(P_i^{k+1} - P_i^k\right) - \left(\frac{\mathcal{E}_{b}{}_i^k \times \rho_i^k}{T_i^k \times \Delta t}\right)\left(T_i^{k+1} - T_i^k\right) - \left(\frac{\left(\frac{\rho_{i+1/2}^k \times K_{p}{}_{i+1/2}^k\left(\left(P_{i+1}^{k+1} - P_i^{k+1}\right)\right)}{\Delta z}\right) - \left(\frac{\rho_{i-1/2}^k \times K_{p}{}_{i-1/2}^k\left(\left(P_i^{k+1} - P_{i-1}^{k+1}\right)\right)}{\Delta z}\right)}{\Delta z}\right) = 0$$

Discretizing the above yields

$$\left(\frac{\mathcal{E}_{b}{}_i^k \times \rho_i^k}{P_i^k \times \Delta t}\right)\left(P_i^{k+1} - P_i^k\right) - \left(\frac{\mathcal{E}_{b}{}_i^k \times \rho_i^k}{T_i^k \times \Delta t}\right)\left(T_i^{k+1} - T_i^k\right) - \frac{\rho_{i+1/2}^k \times K_{p}{}_{i+1/2}^k}{\Delta z^2}\left(P_{i+1}^{k+1} - P_i^{k+1}\right) + \frac{\rho_{i-1/2}^k \times K_{p}{}_{i-1/2}^k}{\Delta z^2}\left(P_i^{k+1} - P_{i-1}^{k+1}\right) = 0$$

For cell 1

$$\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{P_1^k\times\Delta t}\right)\left(P_1^{k+1}-P_1^k\right)-\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{T_1^k\times\Delta t}\right)\left(T_1^{k+1}-T_1^k\right)-\frac{\rho_{1+1/2}^k\times K_{p\,1+1/2}^{\ k}}{\Delta z^2}\left(P_2^{k+1}-P_1^{k+1}\right)+\frac{\rho_{1-1/2}^k\times K_{p\,1-1/2}^{\ k}}{0.5*\Delta z^2}\left(P_1^{k+1}-P_{i-1(LB)}^{k+1}\right)=0$$

LB=Left boundary which is the same as BW=West boundary

$$\left(\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{P_1^k\times\Delta t}\right)+\frac{\rho_{1+1/2}^k\times K_{p\,1+1/2}^{\ k}}{\Delta z^2}+\frac{\rho_{1-1/2}^k\times K_{p\,1-1/2}^{\ k}}{0.5*\Delta z^2}\right)P_1^{k+1}-\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{T_1^k\times\Delta t}\right)T_1^{k+1}-\frac{\rho_{1+1/2}^k\times K_{p\,1+1/2}^{\ k}}{\Delta z^2}P_2^{k+1}=$$
$$\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{P_1^k\times\Delta t}\right)P_1^k-\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{T_1^k\times\Delta t}\right)T_1^k+\frac{\rho_1^k\times K_{p_1}^{\ k}}{0.5\Delta z^2}P_{BW}^{k+1}$$

$$\left(\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{P_1^k\times\Delta t}\right)+\frac{\rho_{1+1/2}^k\times K_{p\,1+1/2}^{\ k}}{\Delta z^2}+\frac{\rho_{1-1/2}^k\times K_{p\,1-1/2}^{\ k}}{0.5*\Delta z^2}\right)P_1^{k+1}-\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{T_1^k\times\Delta t}\right)T_1^{k+1}-\frac{\rho_{1+1/2}^k\times K_{p\,1+1/2}^{\ k}}{\Delta z^2}P_2^{k+1}=$$
$$\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{\Delta t}\right)-\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{\Delta t}\right)+\frac{\rho_1^k\times K_{p_1}^{\ k}}{0.5\Delta z^2}P_{BW}^{k+1}$$

$$\left(\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{P_1^k\times\Delta t}\right)+\frac{\rho_{1+1/2}^k\times K_{p\,1+1/2}^{\ k}}{\Delta z^2}+\frac{\rho_{1-1/2}^k\times K_{p\,1-1/2}^{\ k}}{0.5*\Delta z^2}\right)P_1^{k+1}-\left(\frac{\varepsilon_{b_1}^{\ k}\times\rho_1^k}{T_1^k\times\Delta t}\right)T_1^{k+1}-\frac{\rho_{1+1/2}^k\times K_{p\,1+1/2}^{\ k}}{\Delta z^2}P_2^{k+1}=$$
$$0+\frac{\rho_1^k\times K_{p_1}^{\ k}}{0.5\Delta z^2}P_{BW}^{k+1}$$

For cell nz

$$\left(\frac{\varepsilon_{b_{nz}}^{\ k}\times\rho_{nz}^k}{P_{nz}^k\times\Delta t}\right)\left(P_{nz}^{k+1}-P_{nz}^k\right)-\left(\frac{\varepsilon_{b_{nz}}^{\ k}\times\rho_{nz}^k}{T_{nz}^k\times\Delta t}\right)\left(T_{nz}^{k+1}-T_{nz}^k\right)-\frac{\rho_{nz+1/2}^k\times K_{p\,nz+1/2}^{\ k}}{0.5*\Delta z^2}\left(P_{nz+1(RB)}^{k+1}-P_{nz}^{k+1}\right)+\frac{\rho_{nz-1/2}^k\times K_{p\,nz-1/2}^{\ k}}{\Delta z^2}\left(P_{nz}^{k+1}-P_{nz-1}^{k+1}\right)=0$$

$$\left(\left(\frac{\varepsilon_{b_{nz}}^{\ k}\times\rho_{nz}^k}{P_{nz}^k\times\Delta t}\right)+\frac{\rho_{nz+1}^k\times K_{p_{nz+1}}^{\ k}}{0.5*\Delta z^2}+\frac{\rho_{nz-1}^k\times K_{p_{nz-1}}^{\ k}}{\Delta z^2}\right)P_i^{k+1}-\left(\frac{\varepsilon_{b_{nz}}^{\ k}\times\rho_{nz}^k}{T_{nz}^k\times\Delta t}\right)T_{nz}^{k+1}$$
$$-\frac{\rho_{nz+1/2}^k\times K_{p\,nz+1/2}^{\ k}}{0.5*\Delta z^2}P_{nz+1(RB)}^{k+1}=\left(\frac{\varepsilon_{b_{nz}}^{\ k}\times\rho_{nz}^k}{P_{nz}^k\times\Delta t}\right)P_{nz}^k-\left(\frac{\varepsilon_{b_{nz}}^{\ k}\times\rho_{nz}^k}{T_{nz}^k\times\Delta t}\right)T_{nz}^k$$

$$\left(\left(\frac{{\mathcal{E}_b}_{nz}^{k} \times \rho_{nz}^{k}}{P_{nz}^{k} \times \Delta t}\right) + \frac{\rho_{nz+1}^{k} \times {K_p}_{nz+1}^{k}}{0.5 * \Delta z^2} + \frac{\rho_{nz-1}^{k} \times {K_p}_{nz-1}^{k}}{\Delta z^2}\right) P_{nz}^{k+1} - \left(\frac{{\mathcal{E}_b}_{nz}^{k} \times \rho_{nz}^{k}}{T_{nz}^{k} \times \Delta t}\right) T_{nz}^{k+1}$$

$$- \frac{\rho_{nz+1/2}^{k} \times {K_p}_{nz+1/2}^{k}}{0.5 * \Delta z^2} P_{nz+1(RB)}^{k+1} = 0$$

Temperature Equation

The general energy equation given by equation 14

$$\left((1-\varepsilon_b)C'_p\rho_p+\varepsilon_b\rho_g C_{p,g}\right)\frac{\partial T}{\partial t}+\rho_g C_{p,g}u_z\frac{\partial T}{\partial z}=-\frac{\partial}{\partial z}(Q_Z)+\frac{4U}{d_t}(T_W-T')+S'$$

From equation (16)

$$Q_Z=-k\frac{\partial T}{\partial z}$$

$$(1-\varepsilon_b)C'_p\rho_p\frac{\partial T}{\partial t}+\varepsilon_b\rho_g C_{p,g}\frac{\partial T}{\partial t}+\frac{\partial\rho_g C_{p,g}u_zT}{\partial z}=-\frac{\partial}{\partial z}\left(-k\frac{\partial T}{\partial z}\right)+\frac{4U}{d_t}(T_W-T')+S'$$

Simplifying further

$$(1-\varepsilon_b)C'_p\rho_p\frac{\partial T}{\partial t}+\varepsilon_b C_{p,g}\rho_g\frac{\partial T}{\partial t}+\frac{\partial\rho_g C_{p,g}u_zT}{\partial z}-k\frac{\partial}{\partial z}\left(\frac{\partial T}{\partial z}\right)=\frac{4U}{d_t}(T_W-T')+S'$$

Where the source term is $S'=(1-\varepsilon_b)\rho_{cat}\sum_{k=1}^{n=1}(-\Delta H_{rk})\,(\eta_k R_k)$

$$\frac{(1-\varepsilon_b)C'_p\rho_p+\varepsilon_b C_{p,g}{\rho_g}_i^k}{\Delta t}\left(T_i^{k+1}-T_i^k\right)+\frac{C^k_{p.g(i)}{\rho_g}^k_{(i)}u^k_{z(i+1)}}{\Delta z}T_i^{k+1}-\frac{C^k_{p.g(i-1)}{\rho_g}^k_{(i-1)}u^k_{z(i)}}{\Delta z}T_{i-1}^{k+1}-\left(\frac{\left(\frac{k^k_{(i+1/2)}}{\Delta z}\left(T_{i+1}^{k+1}-T_i^{k+1}\right)\right)-\left(\frac{k^k_{(i-1/2)}}{\Delta z}\left(T_i^{k+1}-T_{i-1}^{k+1}\right)\right)}{\Delta z}\right)=\frac{4U}{d_t}(T_W-T')+S'$$

$$\frac{(1-\varepsilon_b)C'_p\rho_p+\varepsilon_b C_{p,g}{\rho_g}_i^k}{\Delta t}\left(T_i^{k+1}-T_i^k\right)+\frac{C^k_{p.g(i)}{\rho_g}^k_{(i)}u^k_{z(i+1)}}{\Delta z}T_i^{k+1}-\frac{C^k_{p.g(i-1)}{\rho_g}^k_{(i-1)}u^k_{z(i)}}{\Delta z}T_{i-1}^{k+1}-\frac{k^k_{(i+1/2)}\left(T_{i+1}^{k+1}-T_i^{k+1}\right)}{\Delta z^2}+\frac{k^k_{(i-1/2)}\left(T_i^{k+1}-T_{i-1}^{k+1}\right)}{\Delta z^2}=\frac{4U}{d_t}(T_W-T')+(1-\varepsilon_b)\rho_{cat}\sum_{k=1}^{n=1}(-\Delta H_{rk})\,(\eta_k R_k)$$

Simplifying further yields

$$\left(\frac{(1-\varepsilon_b)C'_p\rho_p+\varepsilon_b C_{p,g}{\rho_g}_i^k}{\Delta t}+\frac{C^k_{p.g(i)}{\rho_g}^k_{(i)}u^k_{z(i+1)}}{\Delta z}+\frac{k^k_{(i+1/2)}}{\Delta z^2}+\frac{k^k_{(i-1/2)}}{\Delta z^2}\right)T_i^{k+1}$$
$$-\left(\frac{C^k_{p.g(i-1)}{\rho_g}^k_{(i-1)}u^k_{z(i)}}{\Delta z}+\frac{k^k_{(i-1/2)}}{\Delta z^2}\right)T_{i-1}^{k+1}-\left(\frac{k^k_{(i+1/2)}}{\Delta z^2}\right)T_{i+1}^{k+1}$$
$$=\left(\frac{(1-\varepsilon_b)C'_p\rho_p+\varepsilon_b C_{p,g}{\rho_g}_i^k}{\Delta t}\right)T_i^k+\frac{4U}{d_t}(T_W-T')$$
$$+(1-\varepsilon_b)\rho_{cat}\sum_{k=1}^{n=1}(-\Delta H_{rk})\,(\eta_k R_k)$$

Assuming $k^{k}_{(i+1/2)} = k^{k}_{(i-1/2)}$

$$\left(\frac{(1-\varepsilon_b)C'_p\rho_p + \varepsilon_b C_{p,g}{\rho_g}^k_i}{\Delta t} + \frac{C^k_{p.g(i)}{\rho_g}^k_{(i)}u^k_{z(i+1)}}{\Delta z} + \frac{2k}{\Delta z^2}\right)T^{k+1}_i - \left(\frac{C^k_{p.g(i-1)}{\rho_g}^k_{(i-1)}u^k_{z(i)}}{\Delta z} + \frac{k^k_{(i-1/2)}}{\Delta z^2}\right)T^{k+1}_{i-1} - \left(\frac{k^k_{(i+1/2)}}{\Delta z^2}\right)T^{k+1}_{i+1} = \left(\frac{(1-\varepsilon_b)C'_p\rho_p + \varepsilon_b C_{p,g}{\rho_g}^k_i}{\Delta t}\right)T^k_i + \frac{4U}{d_t}(T_W - T') + (1-\varepsilon_b)\rho_{cat}\sum_{k=1}^{n=1}(-\Delta H_{rk})\,(\eta_k R_k)$$

Where k is the thermal conductivity

For cell 1

$$\frac{(1-\varepsilon_b)C'_p\rho_p + \varepsilon_b C_{p,g}{\rho_g}^k_1}{\Delta t}\left(T^{k+1}_1 - T^k_1\right) + \frac{C^k_{p.g(1)}{\rho_g}^k_{(1)}u^k_{z(1+1/2)}}{\Delta z}T^{k+1}_1 - \frac{C^k_{p.g(1-1)}{\rho_g}^k_{(1-1)}u^k_{z(1)}}{\Delta z}T^{k+1}_{1-1(LB)} - \frac{k^k_{(1+1/2)}\left(T^{k+1}_2 - T^{k+1}_1\right)}{\Delta z^2} + \frac{k^k_{(1-1/2)}\left(T^{k+1}_1 - T^{k+1}_{i-1(LB)}\right)}{0.5*\Delta z^2} = \frac{4U}{d_t}(T_W - T') + (1-\varepsilon_b)\rho_{cat}\sum_{k=1}^{n=1}(-\Delta H_{rk})\,(\eta_k R_k)$$

$$\left(\frac{(1-\varepsilon_b)C'_p\rho_p + \varepsilon_b C_{p,g}{\rho_g}^k_1}{\Delta t} + \frac{C^k_{p.g(1)}{\rho_g}^k_{(1)}u^k_{z((1+1/2))}}{\Delta z} + \frac{3k}{\Delta z^2}\right)T^{k+1}_1 - \left(\frac{k^k_{(i+1/2)}}{\Delta z^2}\right)T^{k+1}_2 = \left(\frac{(1-\varepsilon_b)C'_p\rho_p + \varepsilon_b C_{p,g}{\rho_g}^k_1}{\Delta t}\right)T^k_1 + \frac{4U}{d_t}(T_W - T') + (1-\varepsilon_b)\rho_{cat}\sum_{k=1}^{n=1}(-\Delta H_{rk})\,(\eta_k R_k) + \left(\frac{C^k_{p.g(1-1)}{\rho_g}^k_{(1-1)}u^k_{z(1)}}{\Delta z} + \frac{k^k_{(i-1/2)}}{0.5*\Delta z^2}\right)T^{k+1}_{1-1(LB)}$$

For cell nz

$$\frac{(1-\varepsilon_b)C'_p\rho_p + \varepsilon_b C_{p,g}{\rho_g}^k_{nz}}{\Delta t}\left(T^{k+1}_{nz} - T^k_{nz}\right) + \frac{C^k_{p.g(nz)}{\rho_g}^k_{(nz)}u^k_{z(nz+1/2)}}{\Delta z}T^{k+1}_{nz} - \frac{C^k_{p.g(nz-1)}{\rho_g}^k_{(nz-1)}u^k_{z(nz)}}{\Delta z}T^{k+1}_{nz-1} - \frac{k^k_{(nz+1/2)}\left(T^{k+1}_{nz+1} - T^{k+1}_{nz}\right)}{0.5*\Delta z^2} + \frac{k^k_{(nz-1/2)}\left(T^{k+1}_{nz} - T^{k+1}_{nz-1}\right)}{\Delta z^2} = \frac{4U}{d_t}(T_W - T') + (1-\varepsilon_b)\rho_{cat}\sum_{k=1}^{n=1}(-\Delta H_{rk})\,(\eta_k R_k)$$

Using this boundary condition

At z=L, $\frac{\partial T}{\partial z}=0$

At z=0, $T=T_{in}$

$$\left(\frac{(1-\varepsilon_b)C'_p\rho_p+\varepsilon_b C_{p,g}{\rho_g}^{k}_{nz}}{\Delta t}+\frac{C^k_{p.g(nz)}{\rho_g}^{k}_{(nz)}u^k_{z(nz+1/2)}}{\Delta z}+\frac{k^k_{(nz+1/2)}}{0.5*\Delta z^2}+\frac{k^k_{(nz-1/2)}}{\Delta z^2}\right)T^{k+1}_{nz}$$
$$-\left(\frac{C^k_{p.g(nz-1)}{\rho_g}^{k}_{(nz-1)}u^k_{z(nz)}}{\Delta z}+\frac{k^k_{(nz-1/2)}}{\Delta z^2}\right)T^{k+1}_{nz-1}-\frac{k^k_{(nz+1/2)}}{0.5*\Delta z^2}T^{k+1}_{nz+1}$$
$$=\left(\frac{(1-\varepsilon_b)C'_p\rho_p+\varepsilon_b C_{p,g}{\rho_g}^{k}_{nz}}{\Delta t}\right)T^k_{nz}+\frac{4U}{d_t}(T_W-T')$$
$$+(1-\varepsilon_b)\rho_{cat}\sum_{k=1}^{n=1}(-\Delta H_{rk})\,(\eta_k R_k)$$

Using the exit BC at z=L gives

$$\left(\frac{(1-\varepsilon_b)C'_p\rho_p+\varepsilon_b C_{p,g}{\rho_g}^{k}_{nz}}{\Delta t}+\frac{C^k_{p.g(nz)}{\rho_g}^{k}_{(nz)}u^k_{z(nz+1/2)}}{\Delta z}+\cancel{\frac{k^k_{(nz+1/2)}}{0.5*\Delta z^2}}+\frac{k^k_{(nz-1/2)}}{\Delta z^2}\right)T^{k+1}_{nz}$$
$$-\left(\frac{C^k_{p.g(nz-1)}{\rho_g}^{k}_{(nz-1)}u^k_{z(nz)}}{\Delta z}+\frac{k^k_{(nz-1/2)}}{\Delta z^2}\right)T^{k+1}_{nz-1}-\cancel{\frac{k^k_{(nz+1/2)}}{0.5*\Delta z^2}T^{k+1}_{nz+1}}$$
$$=\left(\frac{(1-\varepsilon_b)C'_p\rho_p+\varepsilon_b C_{p,g}{\rho_g}^{k}_{nz}}{\Delta t}\right)T^k_{nz}+\frac{4U}{d_t}(T_W-T')$$
$$+(1-\varepsilon_b)\rho_{cat}\sum_{k=1}^{n=1}(-\Delta H_{rk})\,(\eta_k R_k)$$

$$\left(\frac{(1-\varepsilon_b)C'_p\rho_p+\varepsilon_b C_{p,g}{\rho_g}^{k}_{nz}}{\Delta t}+\frac{C^k_{p.g(nz)}{\rho_g}^{k}_{(nz)}u^k_{z(nz+1/2)}}{\Delta z}+\frac{k^k_{(nz-1/2)}}{\Delta z^2}\right)T^{k+1}_{nz}$$
$$-\left(\frac{C^k_{p.g(nz-1)}{\rho_g}^{k}_{(nz-1)}u^k_{z(nz)}}{\Delta z}+\frac{k^k_{(nz-1/2)}}{\Delta z^2}\right)T^{k+1}_{nz-1}$$
$$=\left(\frac{(1-\varepsilon_b)C'_p\rho_p+\varepsilon_b C_{p,g}{\rho_g}^{k}_{nz}}{\Delta t}\right)T^k_{nz}+\frac{4U}{d_t}(T_W-T')$$
$$+(1-\varepsilon_b)\rho_{cat}\sum_{k=1}^{n=1}(-\Delta H_{rk})\,(\eta_k R_k)$$

Species Mass Fraction

From equation (4), the species equation is given as

The general form of the species equation is given by

$$\frac{\partial}{\partial t}(\mathcal{E}_b \rho_g w_j) + \frac{\partial}{\partial z}(\rho_g u_z w_j) + \frac{\partial}{\partial z}(\mathcal{E}_b J_j) = S_j$$

Where as

$$J_j = -\rho_g D_{L,j} \frac{\partial w_j}{\partial z}$$

Axial diffusion coefficient is given by

$$D_{L_j} = 0.73 D_{m_j} + \frac{0.5 u_z d_p}{1 + 9.49 D_{m_j} / (u_z d_p)}$$

$\frac{\partial}{\partial t}(\mathcal{E}_b \rho_g w_j) + \frac{\partial}{\partial z}(\rho_g u_z w_j) - \frac{\partial}{\partial z}\left(\mathcal{E}_b \rho_g D_{L,j} \frac{\partial w_j}{\partial z}\right) = S_j$………………..(4.1)

Where the reaction source term, $S_j = (1 - \mathcal{E}_b)\rho_{cat} \sum_{k=1}^{n=1} (\nu_{ik})\,(\eta_k R_k)$

Discretizing equation (4.1)

$$\frac{\mathcal{E}_b \times \rho_{g,i}{}^k}{\Delta t}\left(w_{j,i}^{k+1} - w_{j,i}^k\right) + \frac{\rho_{g,i}{}^k u_{z(i+1/2)}^k w_{j,i}^{k+1}}{\Delta z} - \frac{\rho_{g,i-1}{}^k u_{z(i)}^k w_{j,i-1}^{k+1}}{\Delta z} - \left(\frac{\left(\frac{\mathcal{E}_b \times \rho_{g,i+1}{}^k D_{L(i+1)}^k}{\Delta z}\right)\left(w_{j,i+1}^{k+1} - w_{j,i}^{k+1}\right) - \left(\frac{\mathcal{E}_b \times \rho_{g,i-1}{}^k D_{L(i-1)}^k}{\Delta z}\right)\left(w_{j,i}^{k+1} - w_{j,i-1}^{k+1}\right)}{\Delta z}\right) = S_j \ldots$$

$$\frac{\mathcal{E}_b \times \rho_{g,i}{}^k}{\Delta t}\left(w_{j,i}^{k+1} - w_{j,i}^k\right) + \frac{\rho_{g,i}{}^k u_{z(i+1/2)}^k w_{j,i}^{k+1}}{\Delta z} - \frac{\rho_{g,i-1}{}^k u_{z(i)}^k w_{j,i-1}^{k+1}}{\Delta z} - \left(\frac{\mathcal{E}_b \times \rho_{g,i+1}{}^k D_{L(i+1)}^k}{\Delta z^2}\right)\left(w_{j,i+1}^{k+1} - w_{j,i}^{k+1}\right) + \left(\frac{\mathcal{E}_b \times \rho_{g,i-1}{}^k D_{L(i-1)}^k}{\Delta z^2}\right)\left(w_{j,i}^{k+1} - w_{j,i-1}^{k+1}\right) = S_j$$

$$\left(\frac{\mathcal{E}_b \times \rho_{g,i}{}^k}{\Delta t} + \frac{\rho_{g,i}{}^k u_{z(i+1/2)}^k w_{j,i}^{k+1}}{\Delta z} + \frac{\mathcal{E}_b \times \rho_{g,i+1}{}^k D_{L(i+1)}^k}{\Delta z^2} + \frac{\mathcal{E}_b \times \rho_{g,i-1}{}^k D_{L(i-1)}^k}{\Delta z^2}\right) w_{j,i}^{k+1} - \left(\frac{\rho_{g,i-1}{}^k u_{z(i)}^k}{\Delta z} + \frac{\mathcal{E}_b \times \rho_{g,i-1}{}^k D_{L(i-1)}^k}{\Delta z^2}\right) w_{j,i-1}^{k+1} - \frac{\mathcal{E}_b \times \rho_{g,i+1}{}^k D_{L(i+1)}^k}{\Delta z^2} w_{j,i+1}^{k+1} = \left(\frac{\mathcal{E}_b \times \rho_{g,i}{}^k}{\Delta t}\right) w_{j,i}^k + (1 - \mathcal{E}_b)\rho_{cat} \sum_{k=1}^{n=1} (\nu_{ik})\,(\eta_k R_k)$$

Using the following boundary conditions

At z=L, $\frac{\partial w}{\partial z} = 0$

At z=0, w=w_{in}

For cell 1

$$\frac{\mathcal{E}_b \times \rho_{g,1}{}^{k}}{\Delta t}\left(w_{j,1}^{k+1} - w_{j,1}^{k}\right) + \frac{\rho_{g,1}{}^{k} u_{z(1+1/2)}^{k} w_{j,1}^{k+1}}{\Delta z} - \frac{\rho_{g,1-1}{}^{k} u_{z(1)}^{k} w_{j,1-1(LB)}^{k+1}}{\Delta z} - \left(\frac{\mathcal{E}_b \times \rho_{g,2}{}^{k} D_{L(2)}^{k}}{\Delta z^2}\right)\left(w_{j,2}^{k+1} - w_{j,1}^{k+1}\right) + \left(\frac{\mathcal{E}_b \times \rho_{g,1-1}{}^{k} D_{L(1-1)}^{k}}{0.5 * \Delta z^2}\right)\left(w_{j,1}^{k+1} - w_{j,1-1(LB)}^{k+1}\right) = S_j$$

Grouping liketerms

$$\left(\frac{\mathcal{E}_b \times \rho_{g,1}{}^{k}}{\Delta t} + \frac{\rho_{g,1}{}^{k} u_{z(1+1/2)}^{k}}{\Delta z} + \frac{\mathcal{E}_b \times \rho_{g,2}{}^{k} D_{L(2)}^{k}}{\Delta z^2} + \frac{\mathcal{E}_b \times \rho_{g,1-1}{}^{k} D_{L(1-1)}^{k}}{0.5 * \Delta z^2}\right) w_{j,1}^{k+1} - \left(\frac{\mathcal{E}_b \times \rho_{g,2}{}^{k} D_{L(2)}^{k}}{\Delta z^2}\right) w_{j,2}^{k+1} = \frac{\mathcal{E}_b \times \rho_{g,1}{}^{k}}{\Delta t} w_{j,1}^{k} + \left(\frac{\rho_{g,1-1}{}^{k} u_{z(1/2)}^{k}}{\Delta z} + \frac{\mathcal{E}_b \times \rho_{g,1-1}{}^{k} D_{L(1-1)}^{k}}{0.5 * \Delta z^2}\right) w_{j,1-1(LB)}^{k+1} + (1 - \mathcal{E}_b)\rho_{cat} \sum_{k=1}^{n=1} (\nu_{ik})\left(\eta_k R_k\right)$$

NB: Any parameter to the subscript 1-1 is the parameter value at the boundary .

For cell nz

$$\frac{\mathcal{E}_b \times \rho_{g,nz}{}^{k}}{\Delta t}\left(w_{j,nz}^{k+1} - w_{j,nz}^{k}\right) + \frac{\rho_{g,nz}{}^{k} u_{z(nz+1/2)}^{k} w_{j,nz}^{k+1}}{\Delta z} - \frac{\rho_{g,nz-1}{}^{k} u_{z(nz)}^{k} w_{j,nz-1}^{k+1}}{\Delta z} - \left(\frac{\mathcal{E}_b \times \rho_{g,nz+1}{}^{k} D_{L(nz+1)}^{k}}{0.5 * \Delta z^2}\right)\left(w_{j,nz+1}^{k+1} - w_{j,nz}^{k+1}\right) + \left(\frac{\mathcal{E}_b \times \rho_{g,nz-1}{}^{k} D_{L(nz-1)}^{k}}{\Delta z^2}\right)\left(w_{j,nz}^{k+1} - w_{j,nz-1}^{k+1}\right) = S_j$$

Grouping the above and applying exit BC

$$\left(\frac{\varepsilon_b \times {\rho_{g,nz}}^k}{\Delta t} + \frac{{\rho_{g,nz}}^k u^k_{z(nz+{}^1\!/_2)}}{\Delta z} + \frac{\varepsilon_b \times {\rho_{g,nz+1}}^k D^k_{L(nz+1)}}{0.5 * \Delta z^2} + \frac{\varepsilon_b \times {\rho_{g,nz-1}}^k D^k_{L(nz-1)}}{\Delta z^2}\right) w^{k+1}_{j,nz}$$

$$- \left(\frac{{\rho_{g,nz-1}}^k u^k_{z(nz)}}{\Delta z} + \frac{\varepsilon_b \times {\rho_{g,nz-1}}^k D^k_{L(nz-1)}}{\Delta z^2}\right) w^{k+1}_{j,nz-1}$$

$$- \left(\frac{\varepsilon_b \times {\rho_{g,nz+1}}^k D^k_{L(nz+1)}}{0.5 * \Delta z^2}\right) w^{k+1}_{j,nz+1}$$

$$= \frac{\varepsilon_b \times {\rho_{g,nz}}^k}{\Delta t} w^k_{j,nz} + (1 - \varepsilon_b)\rho_{cat} \sum_{k=1}^{n=1} (\nu_{ik})\,(\eta_k R_k)$$

With BC, the above equation becomes

$$\left(\frac{\varepsilon_b \times {\rho_{g,nz}}^k}{\Delta t} + \frac{{\rho_{g,nz}}^k u^k_{z(nz+{}^1\!/_2)}}{\Delta z} + \cancel{\frac{\varepsilon_b \times {\rho_{g,nz+1}}^k D^k_{L(nz+1)}}{0.5 * \Delta z^2}} + \frac{\varepsilon_b \times {\rho_{g,nz-1}}^k D^k_{L(nz-1)}}{\Delta z^2}\right) w^{k+1}_{j,nz}$$

$$- \left(\frac{{\rho_{g,nz-1}}^k u^k_{z(nz)}}{\Delta z} + \frac{\varepsilon_b \times {\rho_{g,nz-1}}^k D^k_{L(nz-1)}}{\Delta z^2}\right) w^{k+1}_{j,nz-1}$$

$$- \cancel{\left(\frac{\varepsilon_b \times {\rho_{g,nz+1}}^k D^k_{L(nz+1)}}{0.5 * \Delta z^2}\right) w^{k+1}_{j,nz+1}}$$

$$= \frac{\varepsilon_b \times {\rho_{g,nz}}^k}{\Delta t} w^k_{j,nz} + (1 - \varepsilon_b)\rho_{cat} \sum_{k=1}^{n=1} (\nu_{ik})\,(\eta_k R_k)$$

$$\left(\frac{\varepsilon_b \times {\rho_{g,nz}}^k}{\Delta t} + \frac{{\rho_{g,nz}}^k u^k_{z(nz+{}^1\!/_2)}}{\Delta z} + \frac{\varepsilon_b \times {\rho_{g,nz-1}}^k D^k_{L(nz-1)}}{\Delta z^2}\right) w^{k+1}_{j,nz}$$

$$- \left(\frac{{\rho_{g,nz-1}}^k u^k_{z(nz)}}{\Delta z} + \frac{\varepsilon_b \times {\rho_{g,nz-1}}^k D^k_{L(nz-1)}}{\Delta z^2}\right) w^{k+1}_{j,nz-1}$$

$$= \frac{\varepsilon_b \times {\rho_{g,nz}}^k}{\Delta t} w^k_{j,nz} + (1 - \varepsilon_b)\rho_{cat} \sum_{k=1}^{n=1} (\nu_{ik})\,(\eta_k R_k)$$