

Modelo Multifásico

$$\frac{\partial}{\partial t} \left(\varepsilon_k \rho_k \langle \phi_k \rangle^k \right) + \frac{\partial}{\partial x_i} \left(\varepsilon_k \rho_k \langle \phi_k \rangle^k \langle v_k \rangle_i^k \right) = \frac{\partial}{\partial x_i} \left(\varepsilon_k \Lambda_k^* \frac{\partial \langle \Phi_k \rangle^k}{\partial x_i} \right) + \sum_{\substack{j=1 \\ j \neq k}}^n \Theta_{kj}$$

Continuidade:

$$\frac{\partial}{\partial t} (\varepsilon_k \rho_k) + \frac{\partial}{\partial x_i} \left(\varepsilon_k \rho_k \langle v_k \rangle_i^k \right) = \sum_{\substack{j=1 \\ j \neq k}}^n \Gamma_{kj}$$

Energia:

$$\frac{\partial}{\partial t} \left(\varepsilon_k \rho_k \langle h_k \rangle^k \right) + \frac{\partial}{\partial x_i} \left(\varepsilon_k \rho_k \langle h_k \rangle^k \langle v_k \rangle_i^k \right) = \frac{\partial}{\partial x_i} \left(\varepsilon_k K_k^* \frac{\partial \langle T_k \rangle^k}{\partial x_i} \right) + \sum_{\substack{j=1 \\ j \neq k}}^n Q_{kj}$$

Espécies Químicas:

$$\frac{\partial}{\partial t} \left(\varepsilon_k \rho_k \langle C_k \rangle^k \right) + \frac{\partial}{\partial x_i} \left(\varepsilon_k \rho_k \langle C_k \rangle^k \langle v_k \rangle_i^k \right) = \frac{\partial}{\partial x_i} \left(\varepsilon_k D_k^* \frac{\partial \langle C_k \rangle^k}{\partial x_i} \right) + \sum_{\substack{j=1 \\ j \neq k}}^n J_{kj}$$

Discretização:

$$\frac{1}{\Delta t} \left[\left(\varepsilon_k \rho_k \langle \phi_k \rangle^k \right)_{x_i} \right]_t^{t+\Delta t} + \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle \phi_k \rangle^k \langle v_k \rangle_i^k \right)^t \right]_{x_i - \frac{\Delta x_i}{2}}^{x_i + \frac{\Delta x_i}{2}} = \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \Lambda_k^* \frac{\partial \langle \Phi_k \rangle^k}{\partial x_i} \right)^t \right]_{x_i - \frac{\Delta x_i}{2}}^{x_i + \frac{\Delta x_i}{2}} + \sum_{\substack{j=1 \\ j \neq k}}^n \left(\Theta_{kj} \right)_{\bar{x}_i}^t$$

Continuidade:

$$\frac{1}{\Delta t} \left[\left(\varepsilon_k \rho_k \right)_{\bar{x}} \right]_t^{t+\Delta t} + \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle v_k \rangle_i^k \right)^t \right]_{x_i - \delta x_i^-}^{x_i + \delta x_i^+} = \sum_{\substack{j=1 \\ j \neq k}}^n \left(\Gamma_{kj} \right)_{\bar{x}}^t$$

$$\frac{\Delta \left(\varepsilon_k \rho_k \right)_{\bar{x}}^t}{\Delta t} = \sum_{\substack{j=1 \\ j \neq k}}^n \left(\Gamma_{kj} \right)_{\bar{x}}^t - \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle v_k \rangle_i^k \right)^t \right]_{x_i - \delta x_i^-}^{x_i + \delta x_i^+}$$

$$\begin{aligned}
& \frac{1}{\Delta t} \left[\left(\varepsilon_k \rho_k \langle \phi_k \rangle^k \right)_{\bar{x}} \right]_t^{t+\Delta t} = \frac{1}{\Delta t} \left[\left(\varepsilon_k \rho_k \right)_{x_i}^{t+\Delta t} \left(\left(\langle \phi_k \rangle^k \right)_{x_i}^t + \left(\Delta \langle \phi_k \rangle^k \right)_{x_i}^t \right) - \left(\varepsilon_k \rho_k \right)_{x_i}^t \left(\langle \phi_k \rangle^k \right)_{x_i}^t \right] = \\
& = \frac{1}{\Delta t} \left[\left(\left(\varepsilon_k \rho_k \right)_{\bar{x}}^t + \Delta \left(\varepsilon_k \rho_k \right)_{\bar{x}}^t \right) \left(\left(\langle \phi_k \rangle^k \right)_{\bar{x}}^t + \left(\Delta \langle \phi_k \rangle^k \right)_{\bar{x}}^t \right) - \left(\varepsilon_k \rho_k \right)_{\bar{x}}^t \left(\langle \phi_k \rangle^k \right)_{\bar{x}}^t \right] = \\
& = \frac{1}{\Delta t} \left[\left(\varepsilon_k \rho_k \right)_{\bar{x}}^t \left(\Delta \langle \phi_k \rangle^k \right)_{\bar{x}}^t + \Delta \left(\varepsilon_k \rho_k \right)_{\bar{x}}^t \left(\left(\langle \phi_k \rangle^k \right)_{\bar{x}}^t + \left(\Delta \langle \phi_k \rangle^k \right)_{\bar{x}}^t \right) \right] = \\
& = \frac{1}{\Delta t} \left[\left(\varepsilon_k \rho_k \right)_{\bar{x}}^t \left(\Delta \langle \phi_k \rangle^k \right)_{\bar{x}}^t + \Delta t \left(\sum_{\substack{j=1 \\ j \neq k}}^n \left(\Gamma_{kj} \right)_{\bar{x}}^t - \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle v_k \rangle_i^k \right)^t \right]_{x_i - \delta x_i^-}^{x_i + \delta x_i^+} \right) \left(\left(\langle \phi_k \rangle^k \right)_{\bar{x}}^t + \left(\Delta \langle \phi_k \rangle^k \right)_{\bar{x}}^t \right) \right] \\
& \left(\Delta \langle \phi_k \rangle^k \right)_{x_i}^t \left[\frac{\left(\varepsilon_k \rho_k \right)_{x_i}^t}{\Delta t} + \sum_{\substack{j=1 \\ j \neq k}}^n \left(\Gamma_{kj} \right)_{\bar{x}}^t - \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle v_k \rangle_i^k \right)^t \right]_{x_i - \delta x_i^-}^{x_i + \delta x_i^+} \right] + \left(\sum_{\substack{j=1 \\ j \neq k}}^n \left(\Gamma_{kj} \right)_{\bar{x}}^t - \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle v_k \rangle_i^k \right)^t \right]_{x_i - \delta x_i^-}^{x_i + \delta x_i^+} \right) \left(\langle \phi_k \rangle^k \right)_{x_i}^t = \\
& \left[\left(\langle \phi_k \rangle^k \right)_{x_i}^{t+\Delta t} - \left(\langle \phi_k \rangle^k \right)_{x_i}^t \right] \left[\frac{\left(\varepsilon_k \rho_k \right)_{x_i}^t}{\Delta t} + \sum_{\substack{j=1 \\ j \neq k}}^n \left(\Gamma_{kj} \right)_{\bar{x}}^t - \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle v_k \rangle_i^k \right)^t \right]_{x_i - \delta x_i^-}^{x_i + \delta x_i^+} \right] + \left(\sum_{\substack{j=1 \\ j \neq k}}^n \left(\Gamma_{kj} \right)_{\bar{x}}^t - \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle v_k \rangle_i^k \right)^t \right]_{x_i - \delta x_i^-}^{x_i + \delta x_i^+} \right) \left(\langle \phi_k \rangle^k \right)_{x_i}^t = \\
& = \left(\langle \phi_k \rangle^k \right)_{x_i}^{t+\Delta t} \left[\frac{\left(\varepsilon_k \rho_k \right)_{x_i}^t}{\Delta t} + \sum_{\substack{j=1 \\ j \neq k}}^n \left(\Gamma_{kj} \right)_{\bar{x}}^t - \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle v_k \rangle_i^k \right)^t \right]_{x_i - \delta x_i^-}^{x_i + \delta x_i^+} \right] - \frac{\left(\varepsilon_k \rho_k \right)_{x_i}^t}{\Delta t} \left(\langle \phi_k \rangle^k \right)_{x_i}^t \\
& \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle \phi_k \rangle^k \langle v_k \rangle_i^k \right)^t \right]_{x_i - \delta x_i^-}^{x_i + \delta x_i^+} = \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle \phi_k \rangle^k \langle v_k \rangle_i^k \right)_{x_i + \delta x_i^+}^t - \left(\varepsilon_k \rho_k \langle \phi_k \rangle^k \langle v_k \rangle_i^k \right)_{x_i - \delta x_i^-}^t \right] \\
& \frac{1}{\Delta x_i} \left[\left(\varepsilon_k \rho_k \langle v_k \rangle_i^k \right)_{x_i + \delta x_i^+}^t \left(\langle \phi_k \rangle^k \right)_{x_i + \delta x_i^+}^t - \left(\varepsilon_k \rho_k \langle v_k \rangle_i^k \right)_{x_i - \delta x_i^-}^t \left(\langle \phi_k \rangle^k \right)_{x_i - \delta x_i^-}^t \right]
\end{aligned}$$