Supporting information for: Modelling and simulation of CLC using a copper-based oxygen carrier in a double loop circulating fluidized bed reactor system

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Table S1: Closure for turbulent model

Turbulent viscosity
$\mu_g^t = \rho_g C_\mu \frac{k_g^2}{\varepsilon_g}$
Turbulent kinetic energy production?
$S_t = C_b \beta (\vec{v}_s - \vec{v}_g)^2$
Turbulent stress tensor?
$\bar{\bar{\tau}}_t = -\frac{2}{3}\rho_g k_g \bar{\bar{\mathrm{I}}} + 2\mu_g^t \bar{\bar{S}}_g$

Table S2: Empirical parameters for the $\kappa - \varepsilon$ model.

C_μ	σ_0	σ_ε	C_1	C_2	C_b
0.09	1.00	1.30	1.44	1.92	0.25

Table S3: Constitutive equations for internal momentum transfer

Gas phase stress
$\bar{\bar{\tau}}_g = 2\alpha_g \mu_g \bar{\bar{S}}_g$
Solid phase stress
$\bar{\bar{\tau}}_s = -(-p_s + \alpha_s \mu_{B,s} \nabla \cdot \vec{v}_s) - 2\alpha_s \mu_s \bar{\bar{S}}_s$
Deformation rate for phase k ($k = g, s$)
$\bar{\bar{S}}_k = \frac{1}{2}\left(\nabla \vec{v}_k + (\nabla \vec{v}_k)^T\right) - \frac{1}{3}(\nabla \cdot \vec{v}_k)\bar{\bar{\mathrm{I}}}$
Solid phase pressure?
$p_s = \alpha_s \rho_s \Theta_s [1 + 2(1-e)\alpha_s g_0]$
solid bulk viscosity?
$\mu_{B,s} = \frac{4}{3}\alpha_s \rho_s d_p g_0 (1+e)\sqrt{\frac{\Theta_s}{\pi}} + \frac{4}{5}\alpha_s \rho_s d_p g_0 (1+e)$
Solid phase shear viscosity?
$\mu_s = \frac{2\mu_s^{dilute}}{\alpha_s g_0 (1+e)}\left[1 + \frac{4}{5}\alpha_s g_0 (1+e)\right]^2 + \frac{4}{5}\alpha_s \rho_s g_0 (1+e)\sqrt{\frac{\Theta_s}{\pi}}$
Conductivity of the granular temperature?
$\kappa_s = \frac{15}{2}\frac{\mu_s^{dilute}}{(1+e)g_0}\left[1 + \frac{6}{5}\alpha_s g_0 (1+e)\right]^2 + 2\alpha_s^2 \rho_s d_p (1+e) g_0 \sqrt{\frac{\Theta_s}{\pi}}$
Collisional energy dissipation?
$\gamma_s = 3(1-e^2)\alpha_s^2 \rho_s g_0 \Theta_s \left[\frac{4}{d_p}\sqrt{\frac{\Theta_s}{\pi}} - \nabla \cdot \vec{v}_s\right]$
Radial distribution function?
$g_0 = \frac{1 + 2.5\alpha_s + 4.5904\alpha_s^2 + 4.515439\alpha_s^3}{\left[1 - (\frac{\alpha_s}{\alpha_s^{max}})^3\right]^{0.67802}}$
Dilute viscosity?
$\mu_s^{dilute} = \frac{5}{96}\rho_s d_p \sqrt{\pi \Theta_s}$
Interfacial force
$\vec{M}_g = -\vec{M}_s = \beta(\vec{u}_s - \vec{u}_g)$
Drag coefficients?
$\beta = C[\frac{17.3}{Re_p} + 0.336]\frac{\rho_g}{d_s}\lvert\mathbf{v}_s - \mathbf{v}_g\rvert \alpha_s \alpha_g^{-1.8}$

Table S4: Constitutive equations for mass transfer

Effective diffusivity
$D^e_{k,j} = D^m_{k,j} + D^t_k$
Molecular diffusion coefficient?
$D^m_{g,j} = \dfrac{1-\omega_j}{M_m \sum\limits_{j\neq i} \frac{\omega_j}{M_j D_{ji}}}$
Binary diffusion coefficient?
$D_{ji} = \dfrac{T_0^{1.75}\sqrt{1/M_j + 1/M_i}}{101.325P\left((\sum V)_j^{1/3} + (\sum V)_i^{1/3}\right)^2}$
Turbulent diffusion coefficient?
$D^t_g = \dfrac{\mu^t_g}{\rho_g Sc^t}$
$D^t_s = \dfrac{d_p}{16\alpha_s}\sqrt{\pi}\Theta$

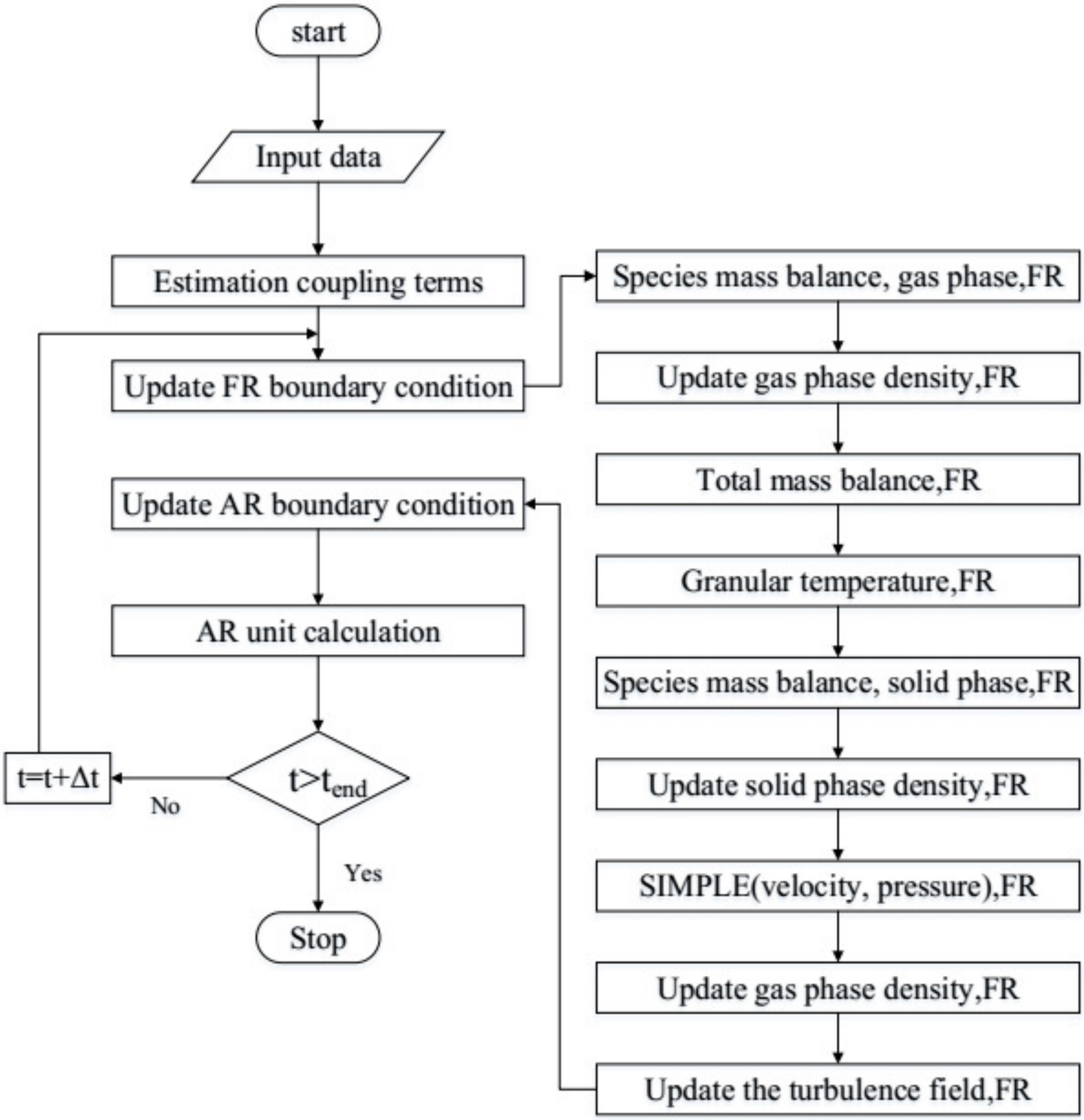

Figure S1: Sketch of the numerical solution algorithm