# Electronic Supplementary Material

# Effect of adjusted mesoscale drag model on flue gas desulfurization in powder-particle spouted beds

**Xinxin Che, Feng Wu (✉), Xiaoxun Ma**

School of Chemical Engineering, Northwest University, Xi'an 710069, China

E-mail: wufeng@nwu.edu.cn

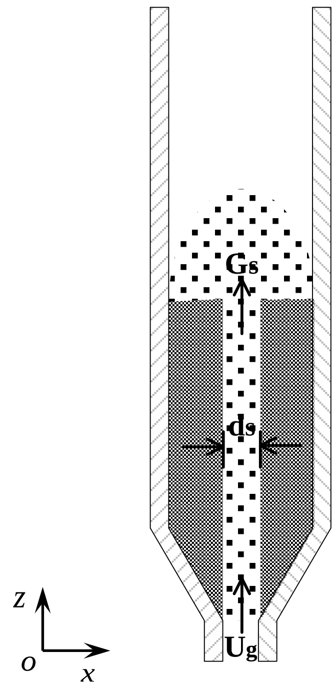


Fig. S1. Schematic diagram of spout structure in spouted bed

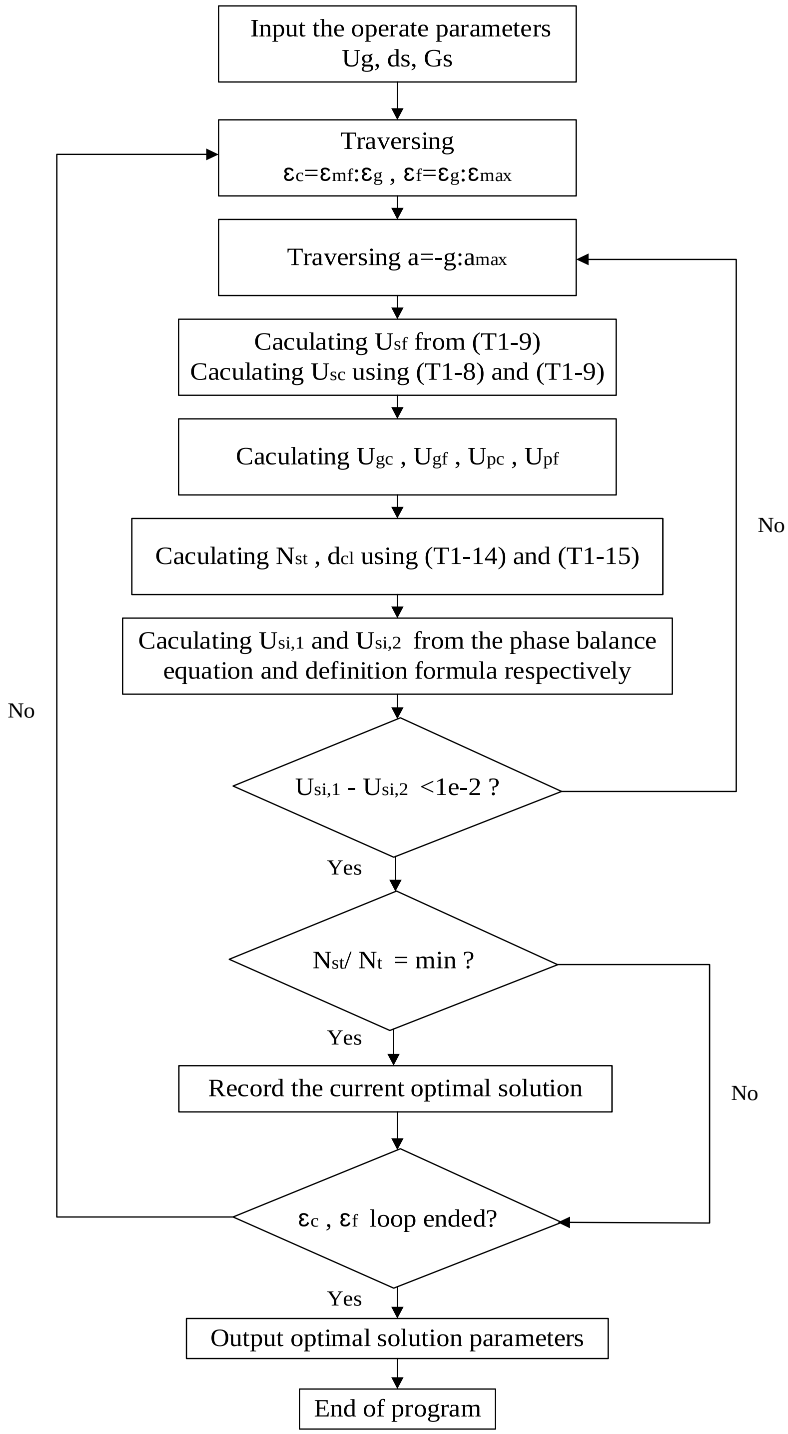



Fig. S2. Flow chart of solving EMMS equations

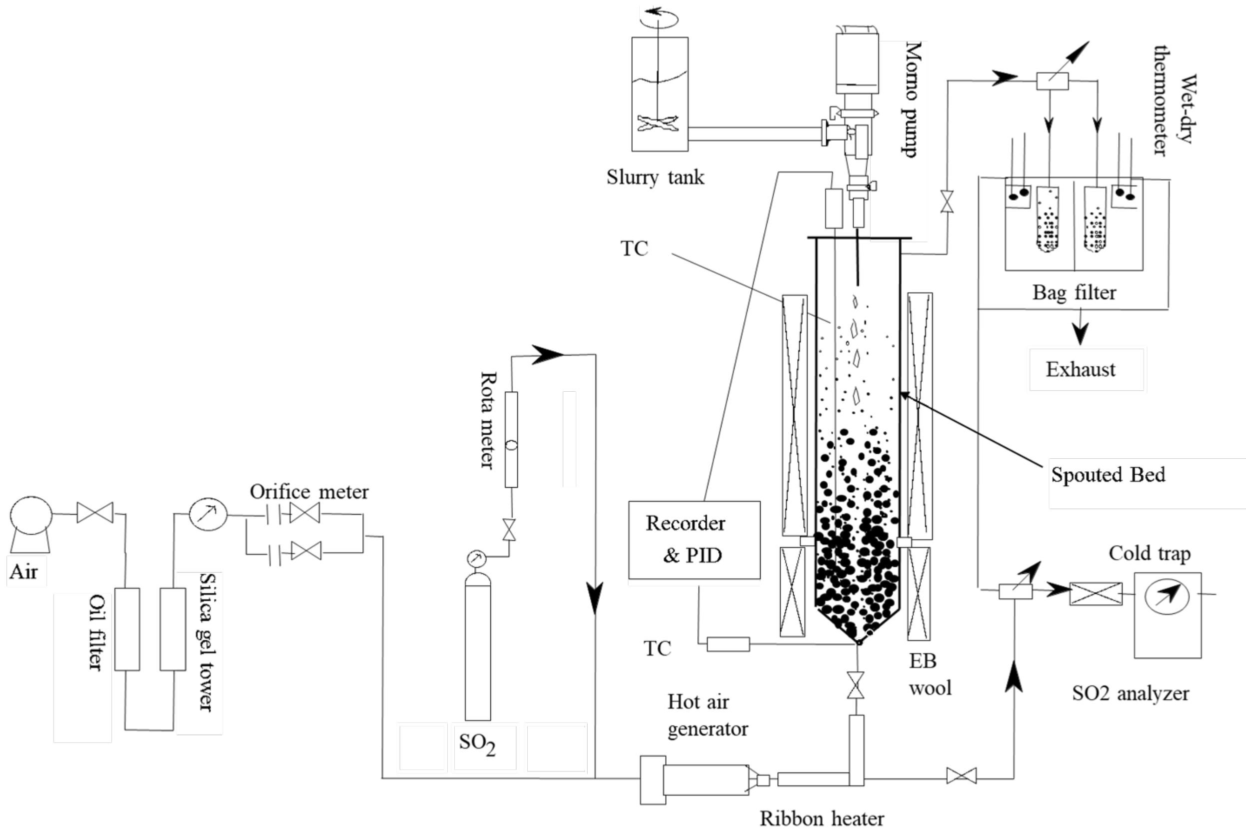
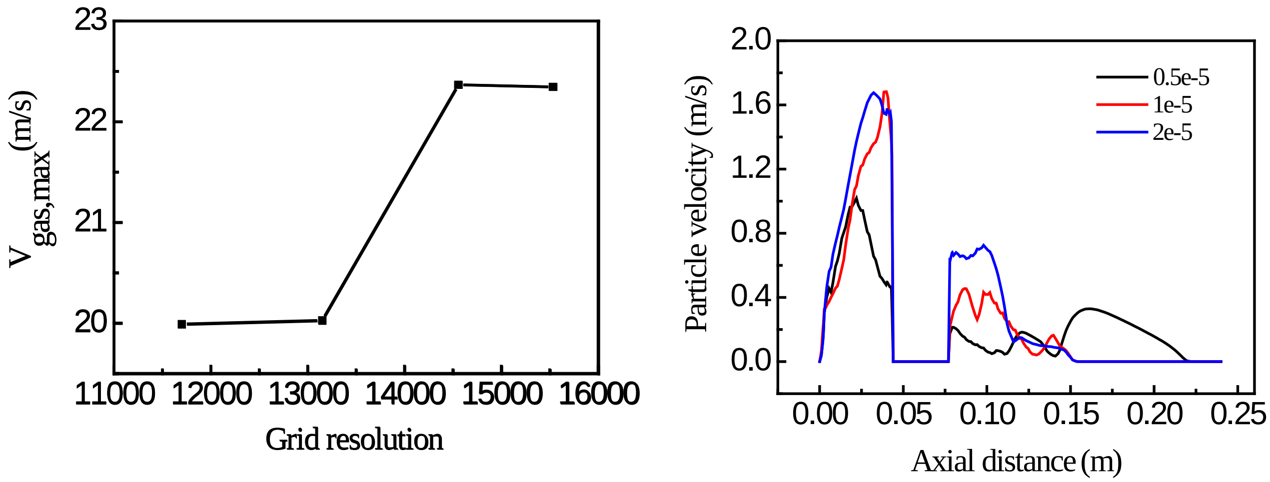



Fig. S3. Schematic diagram of powder-particle spouted bed for semi-dry flue gas desulfurization




(a) Grid independence verification (b) Time step independence verification

Fig. S4. Grid and time step independent verification

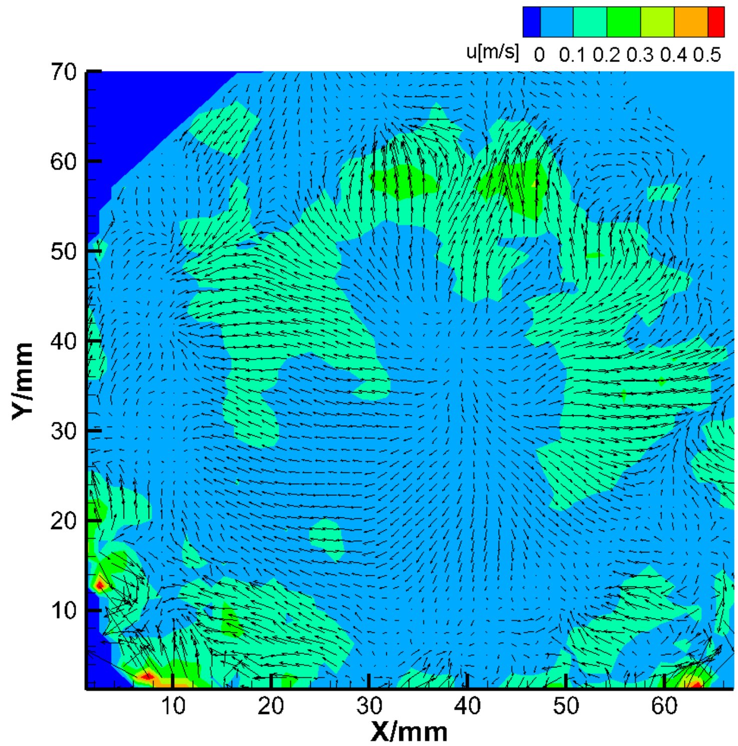



Fig. S5. The contour of the particle radial velocity vector in the spouted bed (z=0.16m)

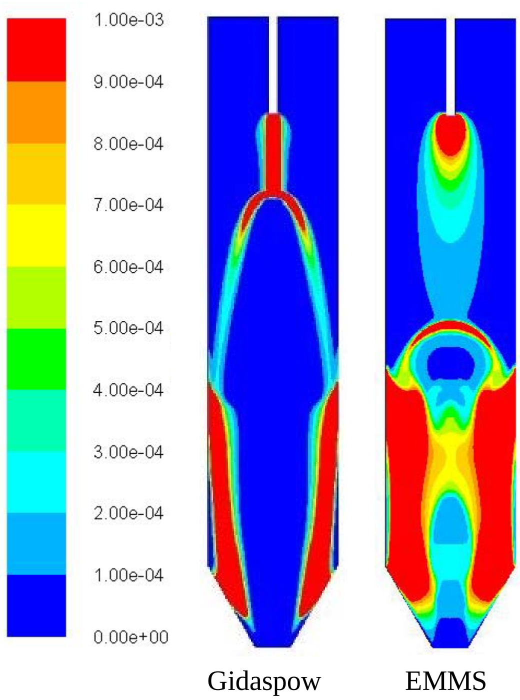



Fig. S6. Contours of water volume fraction under different drag models (T=6.9s)

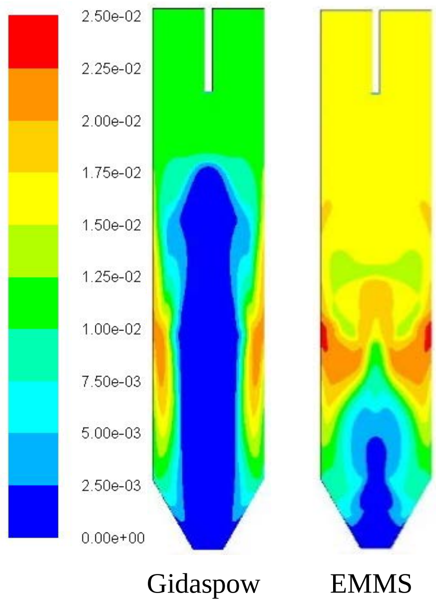



Fig. S7. Contours of mass fraction of $H_2O$ in gas under different drag models

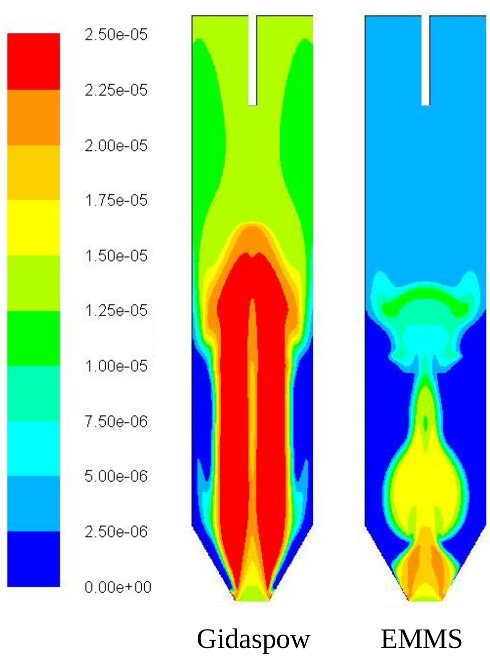



Fig. S8. Contours of $SO_2$ molar concentration under different drag models

Table S1 Governing equation and constitutive relationship of spouted bed

A. Conservation equations

1. Mass conservation equation

$$\frac{\partial}{\partial t}(\varepsilon_\omega \rho_\omega) + \nabla \cdot (\varepsilon_\omega \rho_\omega \vec{v}_\omega) = 0 \qquad \text{(T1-1)}$$

2. Momentum conservation equation

$$\frac{\partial}{\partial t}(\varepsilon_\omega \rho_\omega \vec{v}_\omega) + \nabla \cdot (\varepsilon_\omega \rho_\omega \vec{v}_\omega \vec{v}_\omega) = -\alpha_\omega \nabla P_g + \alpha_\omega \rho_\omega g + \nabla \cdot \overline{\overline{\tau_\omega}} \qquad \text{(T1-2)}$$

3. Energy conservation equation

$$\frac{\partial}{\partial t}\left(\alpha_\omega \rho_\omega \hbar_\omega\right) + \nabla \cdot \left(\alpha_\omega \rho_\omega \vec{v}_\omega \hbar_\omega\right) = -\alpha_\omega \frac{\partial p_\omega}{\partial t} + \bar{\bar{\tau}}: \nabla \vec{v}_\omega - \nabla \cdot \vec{q}_\omega \qquad \text{(T1-3)}$$

4. Component transport equation

$$\frac{\partial}{\partial t}\left(\alpha_\omega \rho_\omega Y_\omega^i\right) + \nabla \cdot \left(\alpha_\omega \rho_\omega Y_\omega^i \vec{v}_\omega\right) = -\nabla \cdot \alpha_\omega \vec{J}_\omega^i + \alpha_\omega R_\omega^i + \alpha_\omega S_\omega^i \qquad \text{(T1-4)}$$

5. Granular temperature equation

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\alpha_\omega \rho_\omega \theta_\omega) + \nabla \cdot (\alpha_\omega \rho_\omega \theta_\omega \vec{v}_\omega)\right] = \left(-\nabla p_\omega \bar{I} + \overline{\overline{\tau_\omega}}\right): \nabla \vec{v}_\omega + \nabla \cdot (k_\omega \nabla \theta_\omega) - \gamma_{\theta_s} - 3\beta\theta_s \qquad \text{(T1-5)}$$

B. Constitutive equations

1. Turbulent kinetic energy equation k

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q k_q\right) + \nabla \cdot \left(\alpha_q \rho_q k_q \overrightarrow{u_q}\right) = \nabla \cdot \left(\alpha_q \frac{\mu_{t,q}}{\sigma_k} \nabla k_q\right) + \alpha_q G_{k,q} - \alpha_q \rho_q \varepsilon_q + \alpha_q \rho_q \prod_{k_q} \qquad \text{(T1-6)}$$

2. Specific dissipation rate equation

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q \varepsilon_q\right) + \nabla \cdot \left(\alpha_q \rho_q \varepsilon_q \overrightarrow{u_q}\right) = \nabla \cdot \left(\alpha_q \frac{\mu_{t,q}}{\sigma_k} \nabla \varepsilon_q\right) + \alpha_q \frac{\varepsilon_q}{k_q}\left(C_{1\varepsilon} G_{k,q} - C_{2\varepsilon} \rho_q \varepsilon_q\right) + \alpha_q \rho_q \prod_{\varepsilon_q} \qquad \text{(T1-7)}$$

Table S2 Hydrodynamic equations of EMMS model

1.Momentum equation of dense phase particles in unit volume microelement:

$$\frac{3}{4}C_{\mathrm{dc}}\frac{f(1-\varepsilon_c)}{d_p}\rho_g U_{sc}^2+\frac{3}{4}C_{\mathrm{di}}\frac{f}{d_{\mathrm{cl}}}\rho_g U_{si}^2=f(1-\varepsilon_c)(\rho_p-\rho_g)(g+a) \quad \text{(T1-8)}$$

2.Momentum equation of dilute particles in unit volume microelement:

$$\frac{3}{4}C_{\mathrm{df}}\frac{(1-f)(1-\varepsilon_f)}{d_p}\rho_g U_{sf}^2=(1-f)(1-\varepsilon_f)(\rho_p-\rho_g)(g+a) \quad \text{(T1-9)}$$

3.Pressure drop balance equation:

$$C_{\mathrm{df}}\frac{(1-\varepsilon_f)}{d_p}\rho_g U_{sf}^2+\frac{f}{1\text{-}f}C_{\mathrm{di}}\frac{1}{d_{\mathrm{cl}}}\rho_g U_{si}^2=C_{\mathrm{dc}}\frac{1-\varepsilon_c}{d_p}\rho_g U_{sc}^2 \quad \text{(T1-10)}$$

4.Mass conservation equation of fluid:

$$U_g=U_{gc}f+U_{gf}(1-f) \quad \text{(T1-11)}$$

5.Particle mass conservation equation:

$$U_p=U_{pc}f+U_{pf}(1-f) \quad \text{(T1-12)}$$

6.Voidage equation:

$$\varepsilon_g=\varepsilon_c\cdot f+\varepsilon_f(1-f) \quad \text{(T1-13)}$$

7.The correlation of cluster:

$$d_{cl}=\frac{d_p\{\frac{U_p}{1-\varepsilon_{max}}-[U_{mf}+\frac{U_p\varepsilon_{mf}}{1-\varepsilon_{mf}}]\}g}{N_{st}\rho_p/(\rho_p-\rho_g)-[U_{mf}+U_p\varepsilon_{mf}/(1-\varepsilon_{mf})]g} \quad \text{(T1-14)}$$

Where $N_{st}=[U_g-\frac{\varepsilon_f-\varepsilon_g}{1-\varepsilon_g}f(1-f)U_f](g+a)\frac{\rho_p-\rho_g}{\rho_g}$ (T1-15)

8.The stability condition:

$$\frac{N_{\mathrm{st}}}{N_T}=\frac{[U_g(1-\varepsilon_g)-fU_f(\varepsilon_f-\varepsilon_g)(1-f)]}{U_g(1-\varepsilon_g)}=min \quad \text{(T1-16)}$$