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[WANGER INSTITUTE FOR SUSTAINABLE ENERGY RESEARCH]

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CFD Simulation of Carbon Dioxide Capture in Advanced in the riser of a Circulating Fluidized Bed System

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Hamid Arastoopour,
H. R. Linden Professor of Energy
and Director of *WISER*

Research Team Members

Hamid Arastoopour

Javad Abbasian

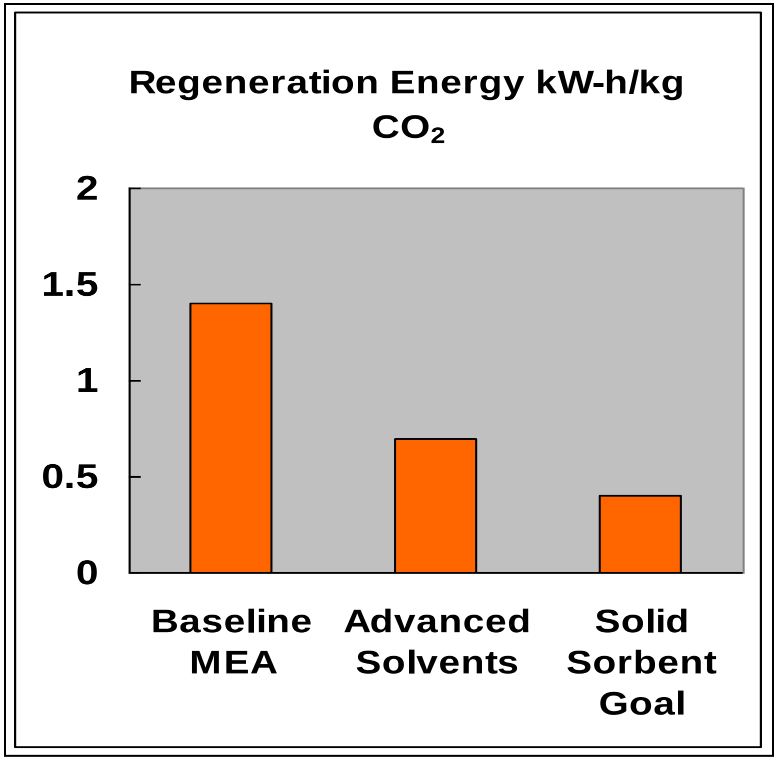
Emad Abbasi (PhD student, Modeling and CFD)

Shahin Zarghami (PhD student, sorbent development and experiments)

Introduction

- **Available processes for CO_2 capture**
  - Pre-combustion CO_2 separation
  - Oxyfuel combustion
  - Post-combustion CO_2 separation
    - Amine based liquid sorbents
    - Membrane separation
    - Cryogenic separation
    - Solid Sorbents

- **Challenges:**
  - Energy Consumption
  - High volume of flue gas
  - low concentration of CO_2

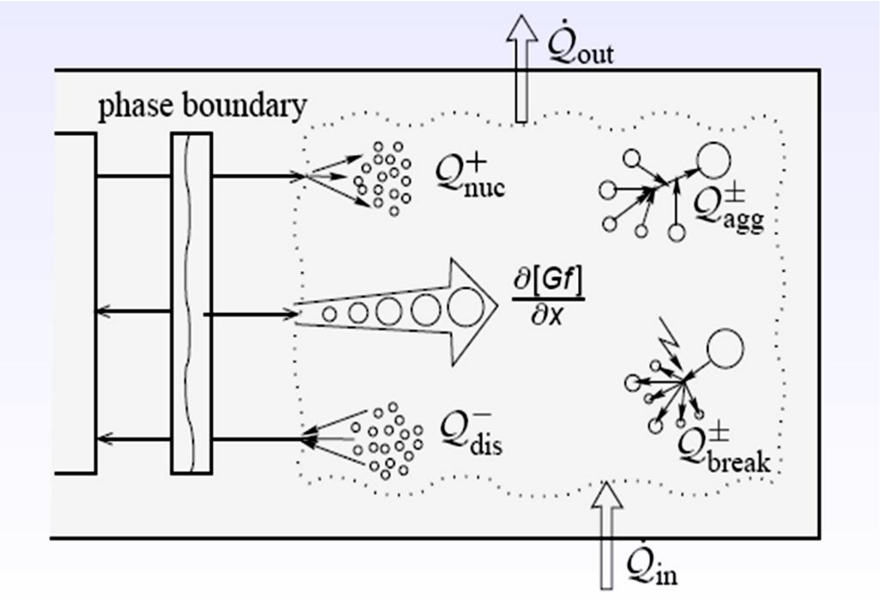


Reported by NETL, 2009

DEVELOPMENT OF A COMPUTATIONAL FLUID DYNAMICS (CFD)/ POPULATION BALANCE (PBE) MODEL

Population Balance Equation

What is the Population Balance Equation?



- **The population balance equation is a balance equation based on the number density function *f (ξ; x, t) with external coordinate x and Internal coordinate ξ .***

- **Accounts for the particles accumulating, leaving, entering or being generated or destroyed in a single control volume**

$$\frac{\partial f(\boldsymbol{\xi};\mathbf{x},t)}{\partial t}+\frac{\partial}{\partial x_i}[u_p(t,\mathbf{x})\,f(\boldsymbol{\xi};\mathbf{x},t)]+\frac{\partial}{\partial x_i}[D_{pt}(\boldsymbol{\xi};\mathbf{x},t)\frac{\partial f(\boldsymbol{\xi};\mathbf{x},t)}{\partial x_i}]+\frac{\partial}{\partial \xi_j}[\frac{\partial \xi_j}{\partial t}\,f(\boldsymbol{\xi};\mathbf{x},t)]=h(\boldsymbol{\xi};\mathbf{x},t)$$

Accumulation term + Convection term + diffusive term + Growth term = Source term

FCMOM

Finite size domain Complete set of trial functions Method Of Moments : FCMOM

- Finite size domain: [-1, 1] instead of [0,∞]
- Solution in terms of both Moments and size distribution
- *f(ξ,x,t)* will be approximated by expansion based on a complete set of trial functions

$$f(\xi, x, t) = \sum_{n=0}^{\infty} C_n(t, x).\Phi_n(\xi) \qquad \text{when} \qquad C_n = \int f(\xi, x, t).\Phi_n(\xi).d\xi$$

$$f(\xi, x, t) = \int [\sum_{m=0}^{\infty} C_m(x, t).\Phi_m(\xi)].\Phi_n(\xi).d\xi$$

set of orthonormal trial functions forming a **complete space**

$$\Phi_0(\xi), \Phi_1(\xi), ..., \Phi_n(\xi)$$

FCMOM

Coordinate Transformation using $\bar{\xi} = \dfrac{\{\xi - [\xi_{\min}(t) + \xi_{\max}(t)]/2\}}{[\xi_{\min}(t) + \xi_{\max}(t)]/2}$

$$\xi \in [0,\infty] \quad \rightarrow \quad \xi \in [\xi_{\min}(t), \xi_{\max}(t)] \quad \rightarrow \quad \bar{\xi} \in [-1,1]$$

Dimensionless distribution function

$$\overline{f'(\bar{\xi},x,t)} = f(\bar{\xi},x,t)/f_{sc}$$

Writing distribution function in terms of series expansion of *Legendre Polynomials*

$$\overline{f'(\bar{\xi},x,t)} \approx \sum_{n=0}^{M-1} c_n(t,x).\phi_n(\bar{\xi})$$

$$c_n = \sqrt{\frac{2n+1}{2}}.\frac{1}{2^n}.\sum_{v=0}^{n}(-1)^{n-v}.\frac{(2v)!}{[(2v-n)!]}.\{\frac{1}{[(n-v)!].[(v)!]}\}.\mu_{2v-n}$$

$$\phi_n(\bar{\xi}) = \sqrt{\frac{2n+1}{2}}.P_n(\bar{\xi})$$

$$P_0(\bar{\xi}) = 1, \quad P_1(\bar{\xi}) = \bar{\xi}, \quad P_2(\bar{\xi}) = \frac{3}{2}\cdot\bar{\xi}^2 - \frac{1}{2},$$

$$P_3(\bar{\xi}) = \frac{5}{2}\cdot\bar{\xi}^3 - \frac{3}{2}\cdot\bar{\xi}, \quad P_4(\bar{\xi}) = \frac{35}{8}\cdot\bar{\xi}^4 - \frac{15}{4}\cdot\bar{\xi}^2 + \frac{3}{8}$$

Moments Transport Equation

$$\mu_i = \int_{-1}^{1} \overline{f}'.(\overline{\xi})^i.d\overline{\xi}$$

$$\frac{\partial \mu_i}{\partial t} + \mu_i \frac{\partial v_{p,j}}{\partial x_j} + v_{p,j} \frac{\partial \mu_i}{\partial x_j} - \frac{\partial}{\partial x_j}\left[\int_{-1}^{+1} D'_{pt} \frac{\partial \overline{f'}}{\partial x_j} (\overline{\xi})^i d\overline{\xi}\right] = -(MB + MB_{Conv} + MB_{Diff1} + MB_{Diff2} + MB_{Diff3} + IG)$$

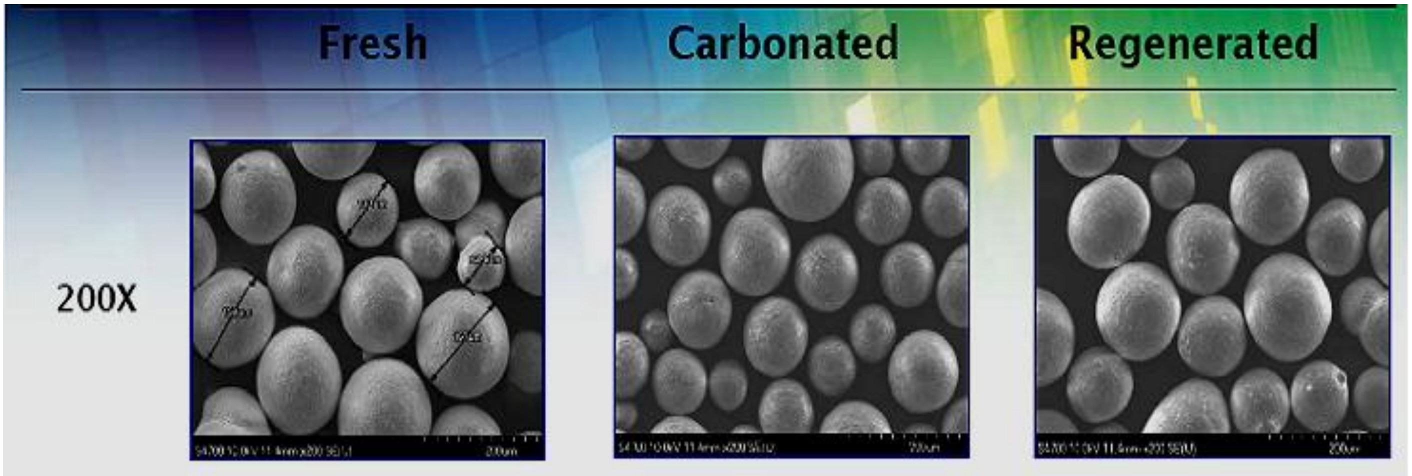
MB : Terms due to coordinate transformation (Moving Boundary)

IG: Contribution due to the Integration of Particle Growth Term

$$IG = \frac{2}{(\xi_{\max} - \xi_{\min})}.\{[G'_{+1}\overline{f'_{+1}} - (-1)^i.G'_{-1}\overline{f'_{-1}}] - i.\int_{-1}^{1} G'\,\overline{f'}.(\overline{\xi})^{i-1}.d\overline{\xi}\}$$

$$G' = \frac{d\overline{\xi}}{dt}$$

CO2 Capture process using solid sorbents



- Particle Size distribution remains unchanged
- Density distribution is changing $f(\xi;\mathbf{x},t)$ where ξ : particle density
- PBE accounts for particle density Distribution changes
- No Birth or Death term for density

$$\frac{\partial f(\xi;\mathbf{x},t)}{\partial t}+\frac{\partial}{\partial x_i}[u_p(t,\mathbf{x})f(\xi;\mathbf{x},t)]+\frac{\partial}{\partial x_i}[D_{pt}(\xi;\mathbf{x},t)\frac{\partial f(\xi;\mathbf{x},t)}{\partial x_i}]+\frac{\partial}{\partial \xi}[\frac{\partial \xi}{\partial t}f(\xi;\mathbf{x},t)]=\cancelto{0}{h(\xi;\mathbf{x},t)}$$

Possible Assumptions

$$\frac{\partial \mu_i}{\partial t} + \mu_i \frac{\partial v_{p,j}}{\partial x_j} + v_{p,j} \frac{\partial \mu_i}{\partial x_j} - \frac{\partial}{\partial x_j}[\int_{-1}^{+1} D'_{pt} \frac{\partial \overline{f'}}{\partial x_j} (\bar{\xi})^i d\bar{\xi}] = -(MB + MB_{Conv} + MB_{Diff1} + MB_{Diff2} + MB_{Diff3} + IG)$$

1-No Birth or Death term for density: Source term is Zero

2- Incompressible particulate phase: $\mu_i \frac{\partial v_{p,j}}{\partial x_j} = 0$

3- Particle Turbulent Diffusivity functionality $D_{pt}=D_{pt}(\xi,x,t)$

- if Homogenous, $D_{pt=} D_{pt}(\xi,,t)$: $MB_{Diff\ 1}$ is Zero
- if density independent, $D_{pt=} D_{pt}(x,t)$: $MB_{Diff\ 3}$ is Zero

4- if $\xi_{min} = \rho_{fresh\ sorbent}$ and $\xi_{max} = \rho_{sorbent\ 100\%\ conversion}$

then all the MB, MB_{conv}, $MB_{Diff\ 1}$, $MB_{Diff\ 2}$, $MB_{Diff\ 3}$ are Zero

we are not dealing with a moving boundary problem nymore

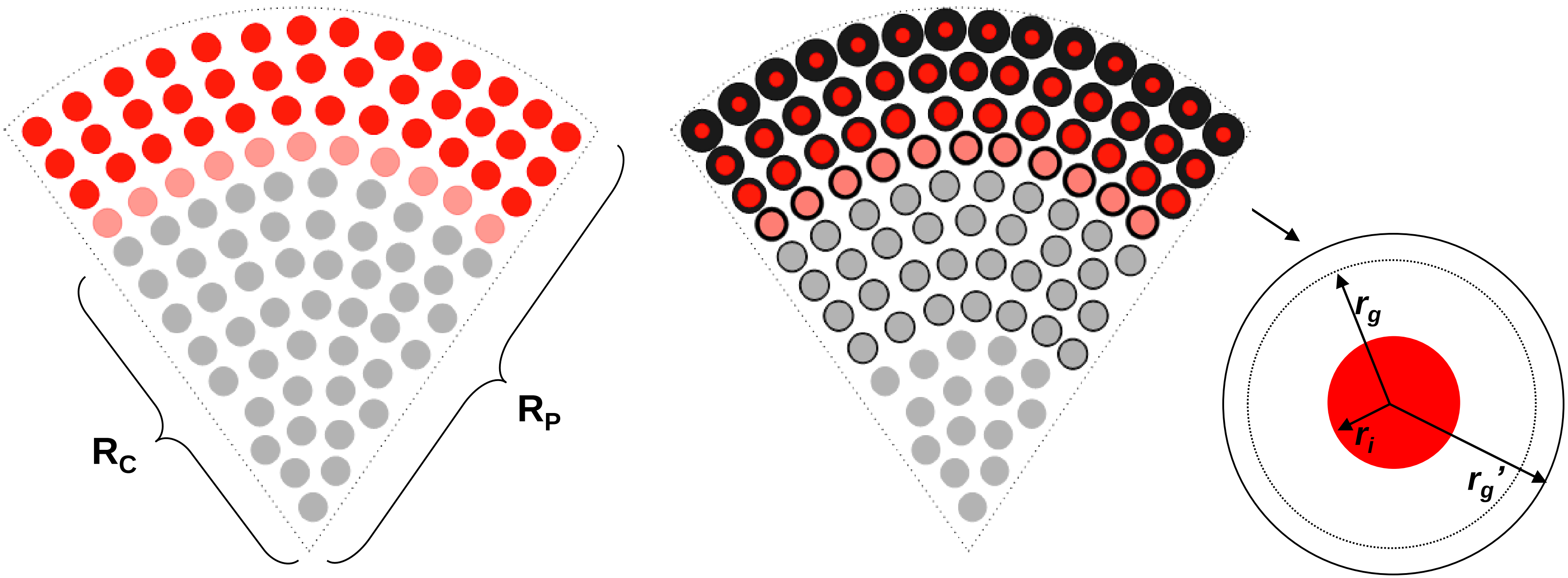
Final PBE Equation

$$\frac{\partial \mu_i}{\partial t} + \frac{\partial}{\partial x_j}[v_{p,j}\mu_i - D'_{pt}(\bar{\xi}, x, t)\frac{\partial \mu_i}{\partial x_j}] =$$

$$-\frac{2}{(\xi_{\max} - \xi_{\min})}.\{[G'_{+1}\overline{f'_{+1}} - (-1)^i.G'_{-1}\overline{f'_{-1}}] - i.\int_{-1}^{1} G'\overline{f'}.(\bar{\xi})^{i-1}.d\bar{\xi}\}$$

Two-Zone Expanding Grain Model

Desired Particle Size about 150 Micron

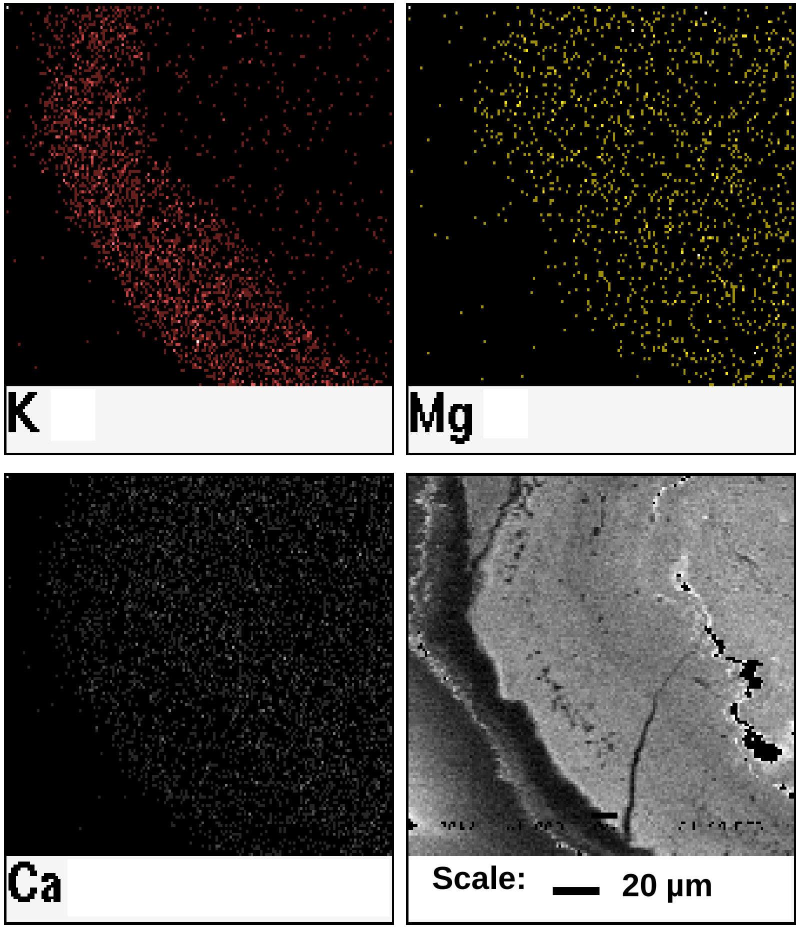


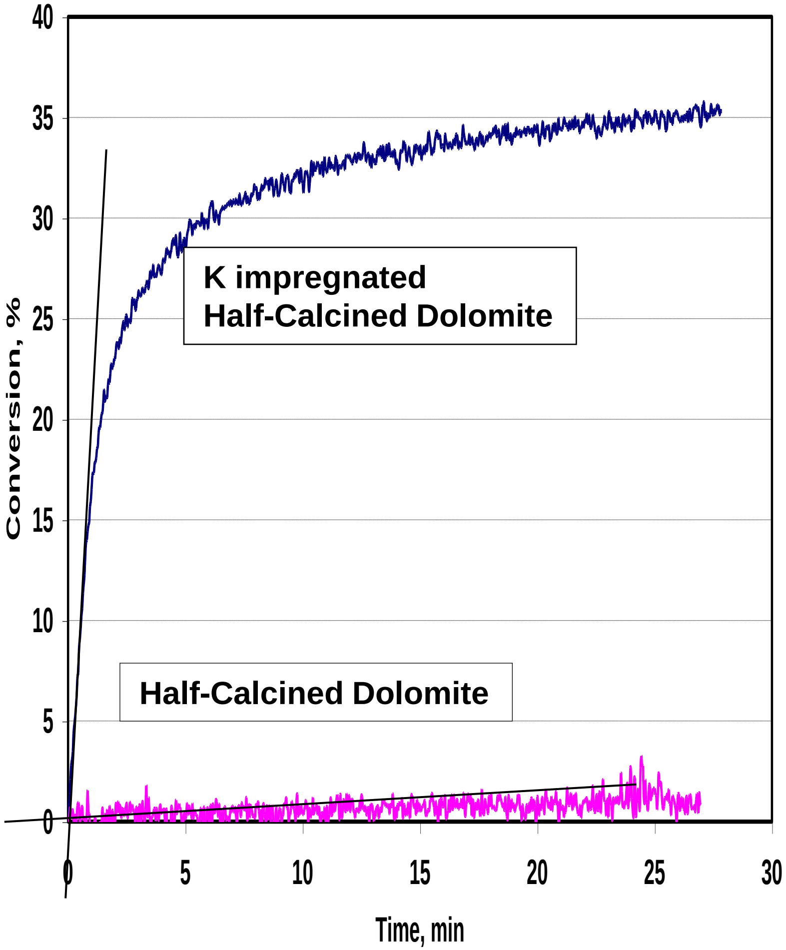
a: Non-Reacted Particle **b: Reacted Particle**

R_P: Radius of Particle
R_C: Radius of Inner Layer

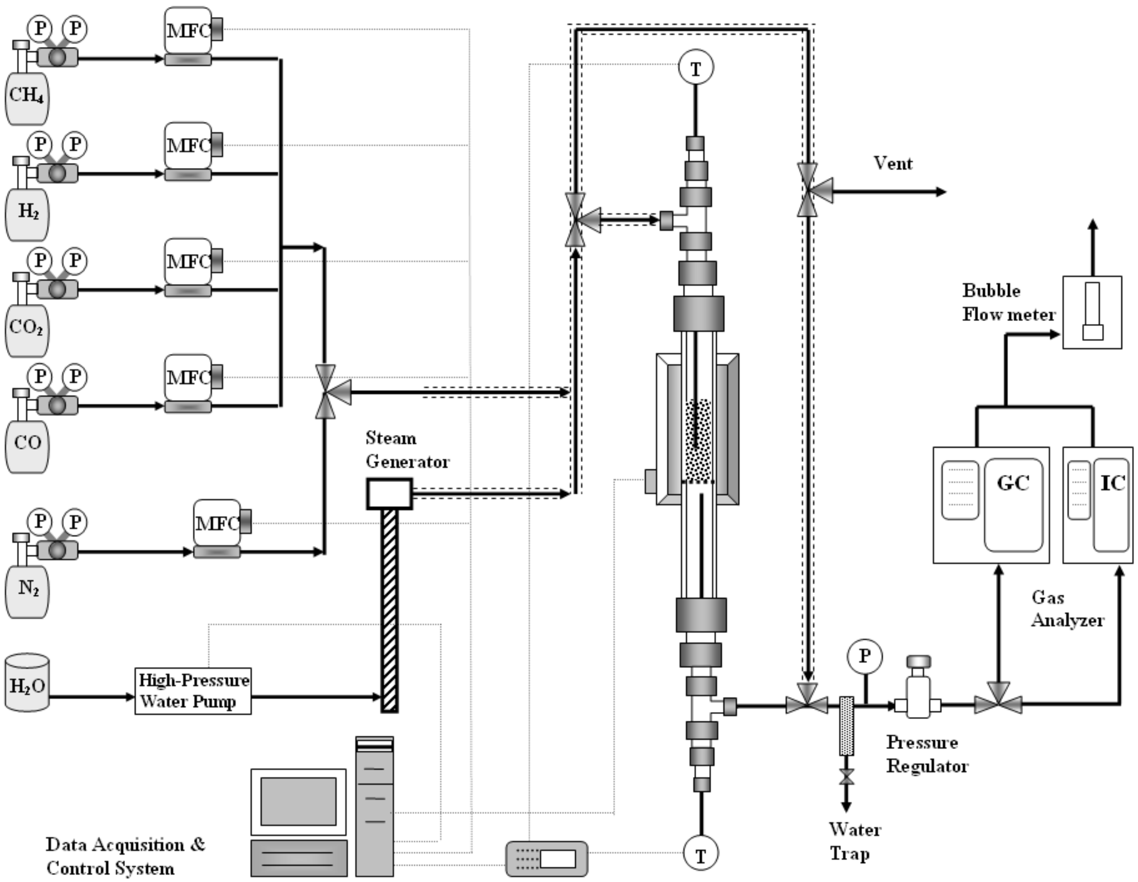
r_i : The radius of the unreacted core of the grain
r_g : Initial radius of the grains
r_g': The radius of the expanded grain

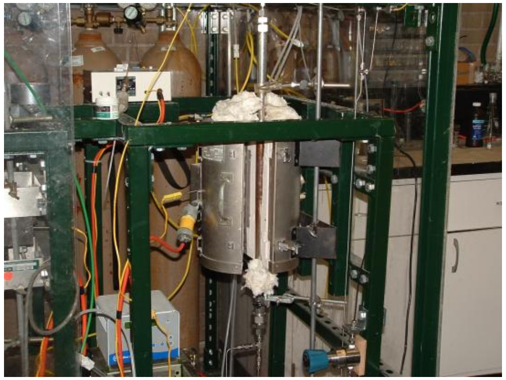
SEM/EDS Results





Modification of High-Pressure Packed Bed

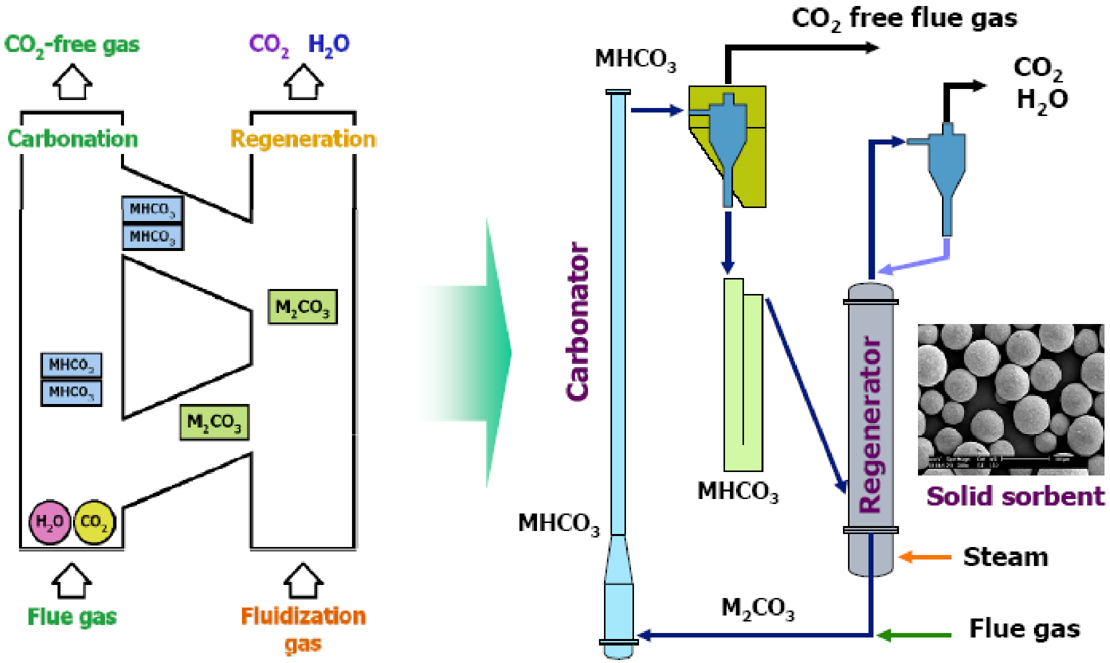




COMPUTATIONAL FLUID DYNAMICS (CFD) SIMULATION OF CO_2 SORPTION IN THE RISER SECTION OF CFB

Objective and Process Concept

Objective: **To validate our CFD model for CO_2 Capture process with solid sorbents in the riser section of a circulating fluidized bed using available experimental data from Korea Institute for Energy Research (KIER).**

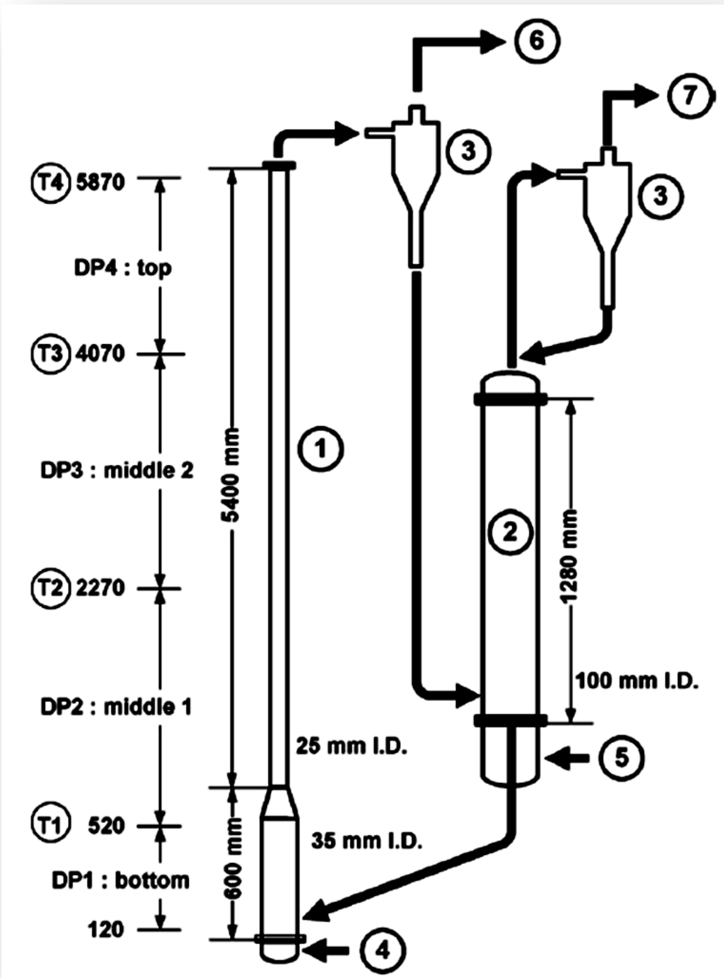


Yi et al., 2007

Carbonation: $CO_2 + H_2O + K_2CO_3 \rightarrow 2KHCO_3 + Heat$

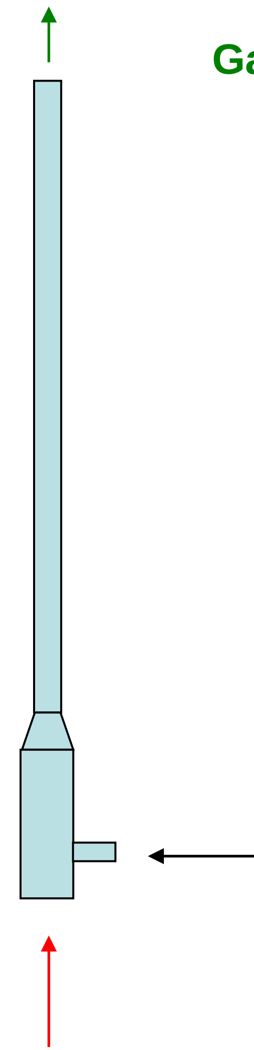
Regeneration: $2KHCO_3 \rightarrow CO_2 + H_2O + K_2CO_3 - Heat$

Experimental setup (KIER, 2007)



Temperature

80°C



Gas-solid outlet

P = 1 atm

Gas inlet

V_g = 2 m/s

10% CO_2

15% H_2O

75% N_2

solid inlet

G_s = 21 kg/m2.s

ε_s = 0.6

35% K_2CO_3

65% inert

0% $KHCO_3$

2D, Eulerian- Eulerian Approach in combination with the kinetic theory of granular flow

- Conservation of Mass

- gas phase: $$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla.(\varepsilon_g \rho_g v_g) = \dot{m}_g$$

- solid phase $$\frac{\partial}{\partial t}(\varepsilon_s \rho_s) + \nabla.(\varepsilon_s \rho_s v_s) = \dot{m}_s$$

- Conservation of Momentum

- gas phase: $$\frac{\partial}{\partial t}(\varepsilon_g \rho_g v_g) + \nabla.(\varepsilon_g \rho_g v_g v_g) = -\varepsilon_g \nabla P + \nabla.\tau_g + \varepsilon_g \rho_g g - \beta_{gs}(v_g - v_s)$$

- solid phase $$\frac{\partial}{\partial t}(\varepsilon_s \rho_s v_s) + \nabla.(\varepsilon_s \rho_s v_s v_s) = -\varepsilon_s \nabla P - \nabla P_s + \nabla.\tau_s + \varepsilon_s \rho_s g + \beta_{gs}(v_g - v_s)$$

Numerical Modeling:
Conservation Equations

- **Conservation of Species**
  - **gas phase:**

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g y_i) + \nabla.(\varepsilon_g \rho_g v_g y_i) = R_j$$

  - **solid phase**

$$\frac{\partial}{\partial t}(\varepsilon_s \rho_s y_i) + \nabla.(\varepsilon_s \rho_s v_s y_i) = R_j$$

- **Conservation of solid phase fluctuating Energy**
  - **solid phase**

$$\frac{3}{2}[\frac{\partial}{\partial t}(\varepsilon_s \rho_s \theta) + \nabla.(\varepsilon_s \rho_s \theta) v_s] = (-\nabla p_s I + \tau_s) : \nabla v_s + \nabla.(\kappa_s \nabla \theta) - \gamma_s$$

Generation of energy due to solid stress tensor | **Diffusion** | **dissipation**

Numerical Modeling:
Drag Correlation

Gas-solid inter-phase exchange coefficient: EMMS model (*Wang et al. 2004)*

$$\beta_{sg} = \begin{cases} \dfrac{3}{4}\dfrac{(1-\varepsilon_g)\varepsilon_g}{d_p}\rho_g\left|u_g - u_s\right| C_{D0}\,\omega(\varepsilon_g) & \varepsilon_g > 0.74 \\ 150\dfrac{(1-\varepsilon_g)^2\mu_g}{\varepsilon_g d_p^{\,2}} + 1.75\dfrac{(1-\varepsilon_g)\rho_g\left|u_g - u_s\right|}{d_p} & \varepsilon_g < 0.74 \end{cases}$$

Heterogeneity Factor

ω < 1

$$\omega(\varepsilon_g) = \begin{cases} -0.5760 + \dfrac{0.0214}{4(\varepsilon_g - 0.7463)^2 + 0.0044} & 0.74 < \varepsilon_g \le 0.82 \\ -0.0101 + \dfrac{0.0038}{4(\varepsilon_g - 0.7789)^2 + 0.0040} & 0.82 < \varepsilon_g \le 0.97 \\ -31.8295 + 32.8295\,\varepsilon_g & \varepsilon_g > 0.97 \end{cases}$$

Accounts for cluster formation by multiplying the “Wen &Yu” drag correlation with a heterogeneity factor

Reaction Kinetic:

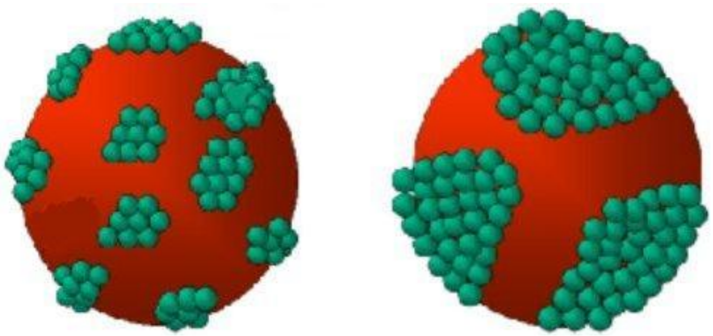
Deactivation Kinetic Model

Carbonation: $CO_2 + H_2O + K_2CO_3 \rightarrow 2KHCO_3 + Heat$

$$-Q_g \frac{dC_{CO_2}}{dA} = kC_{H_2O}C_{CO_2}a \qquad -\frac{da}{dt} = k_d C_{CO_2} a$$

$$a = \exp\left[\frac{[1-\exp(\tau.k_s(1-\exp(-k_d t)))]}{1-\exp(-k_d t)}\exp(-k_d t)\right]$$

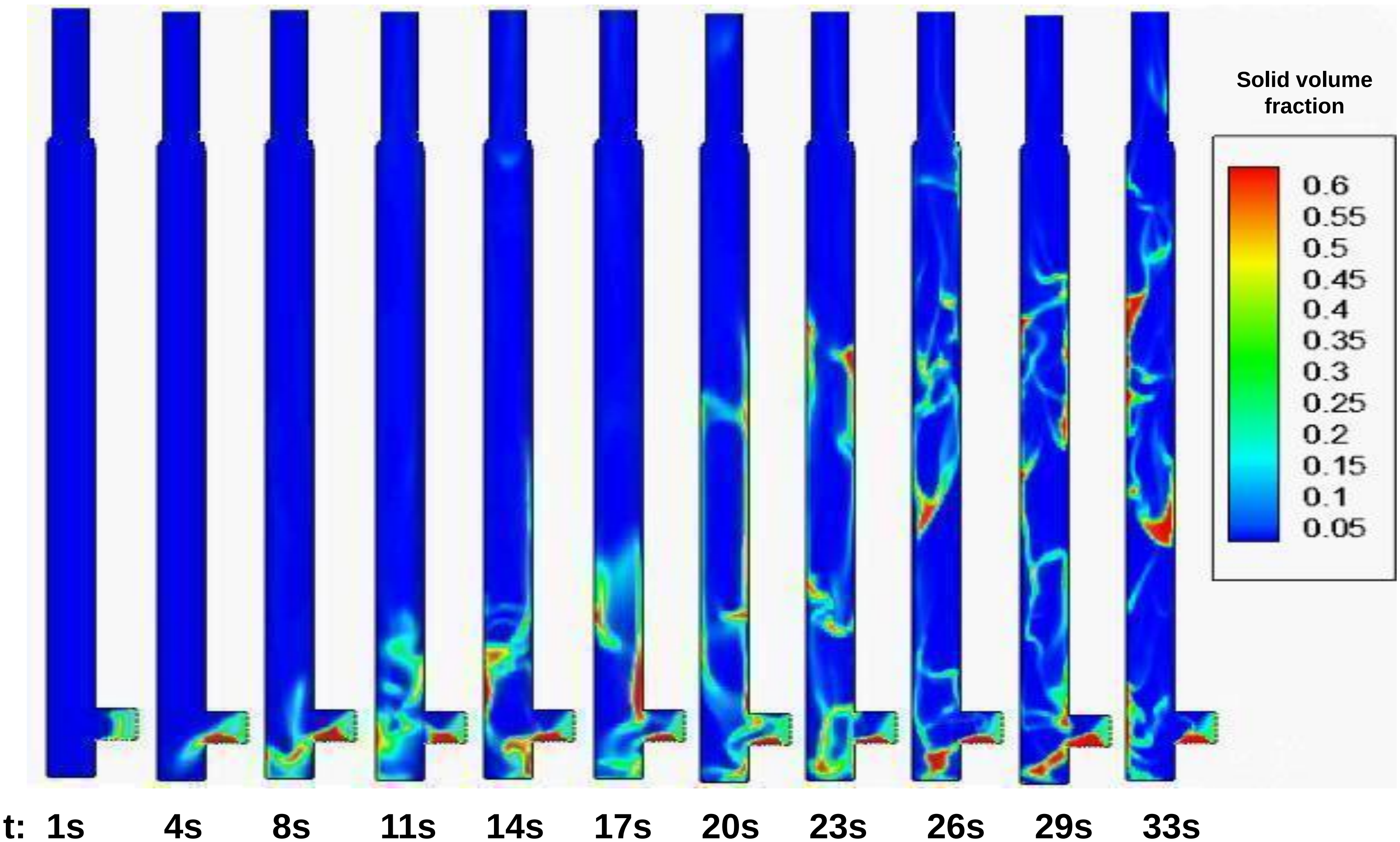
- Proposed by Park et al (2006)



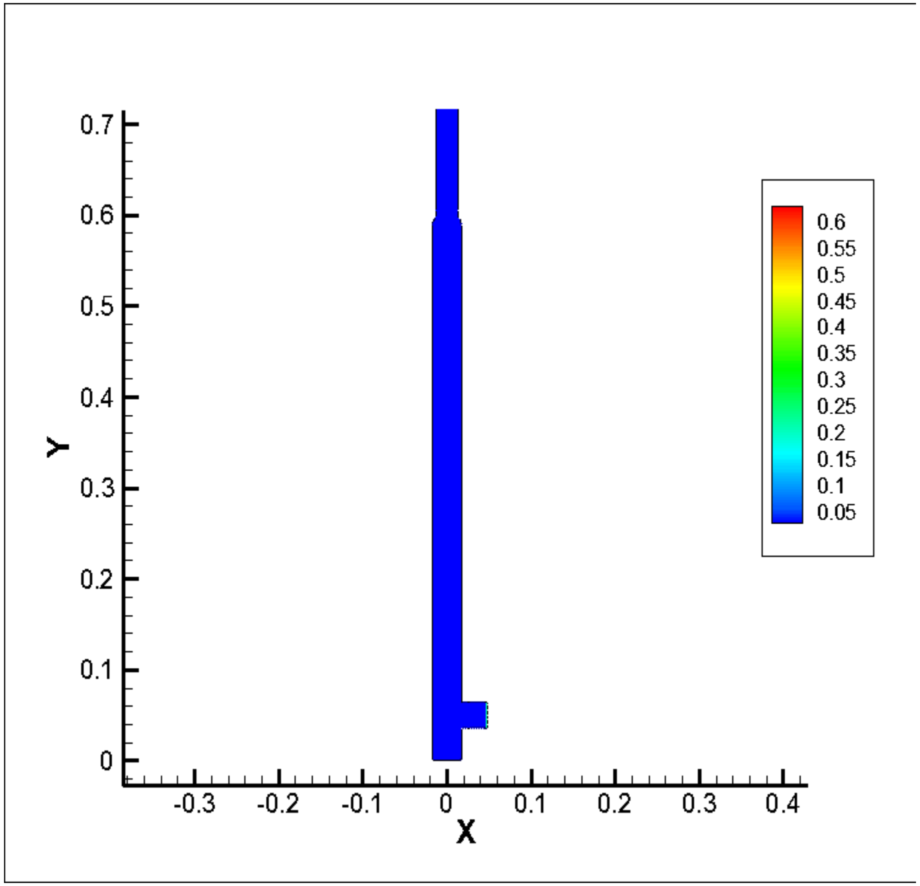
- Compared the result with Homogenous Model: Garg et al. (2010)

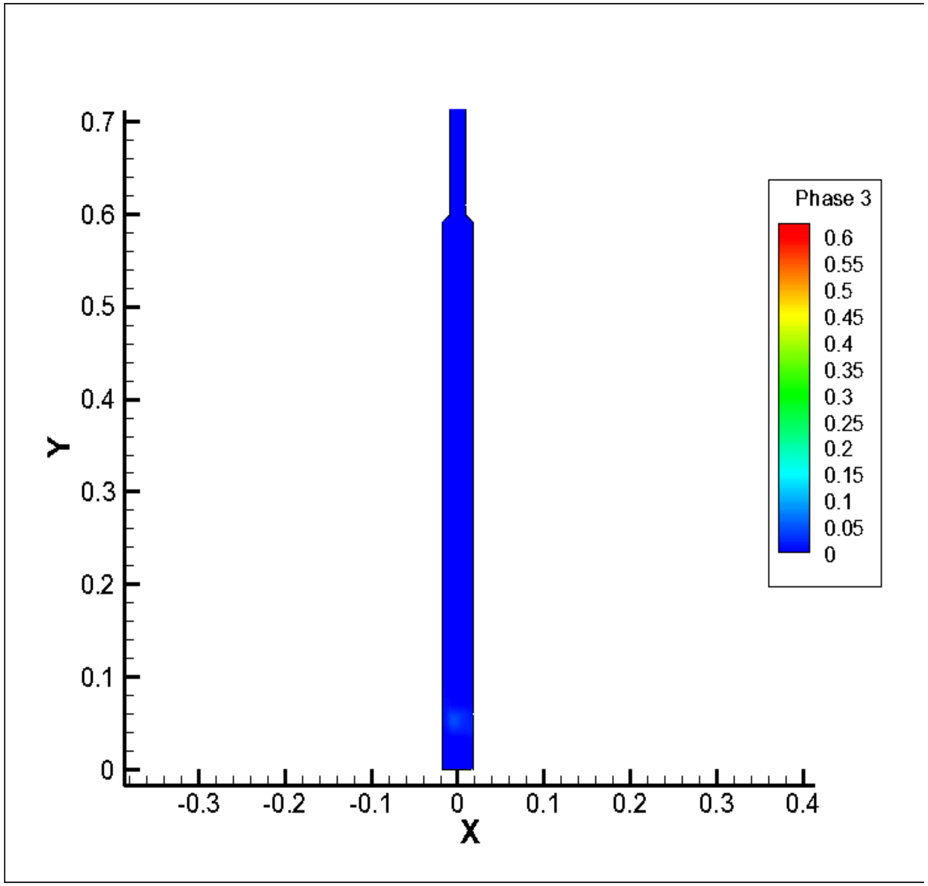
$$-\frac{dC_{CO_2}}{dt} = k\varepsilon_s C_{K_2CO_3} C_{CO_2}$$

Time evolution of Solid Volume Fraction inside the riser

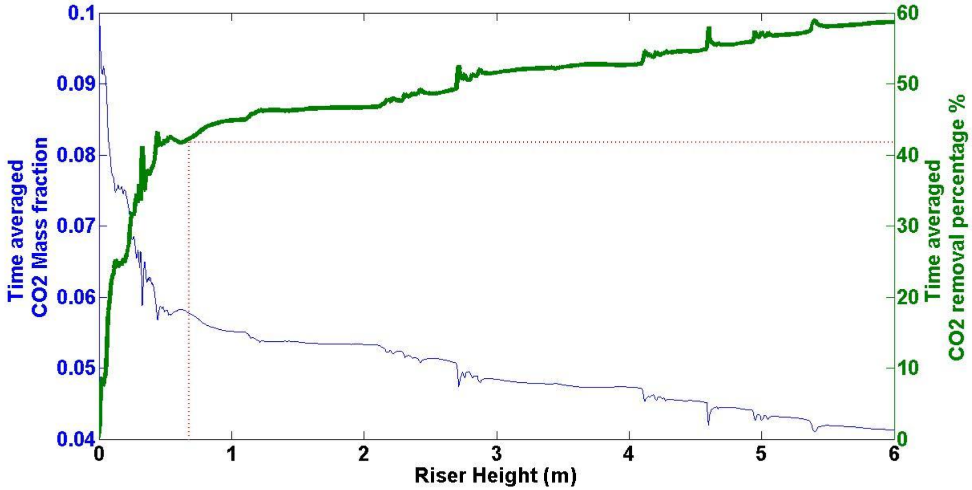


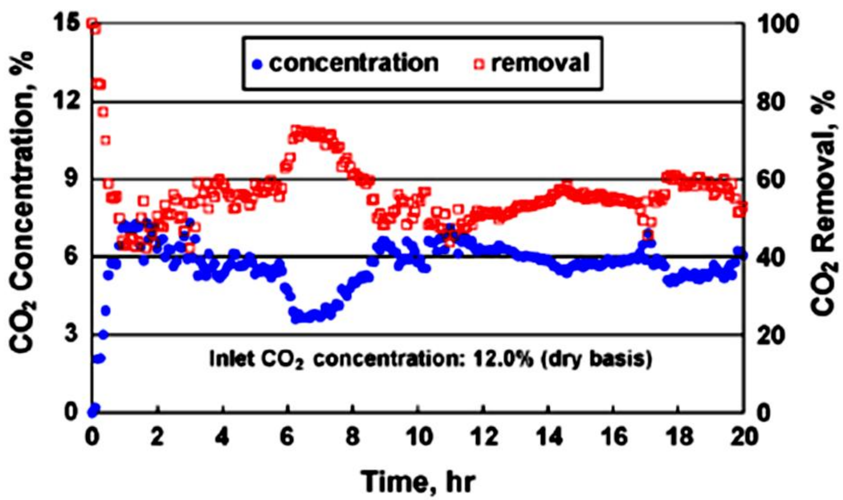
Time evolution of Solid Volume Fraction inside the riser





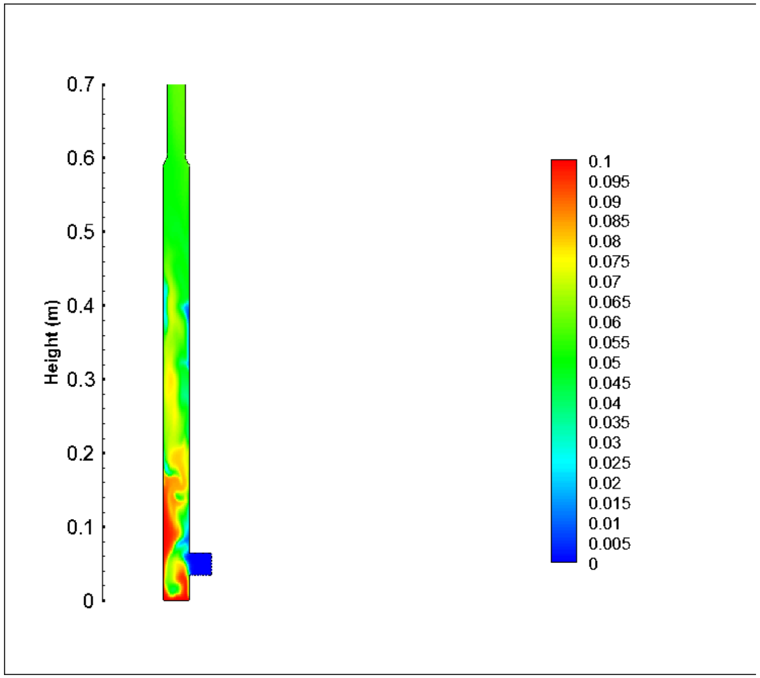
CO_2 Removal





Yi et al., 2007

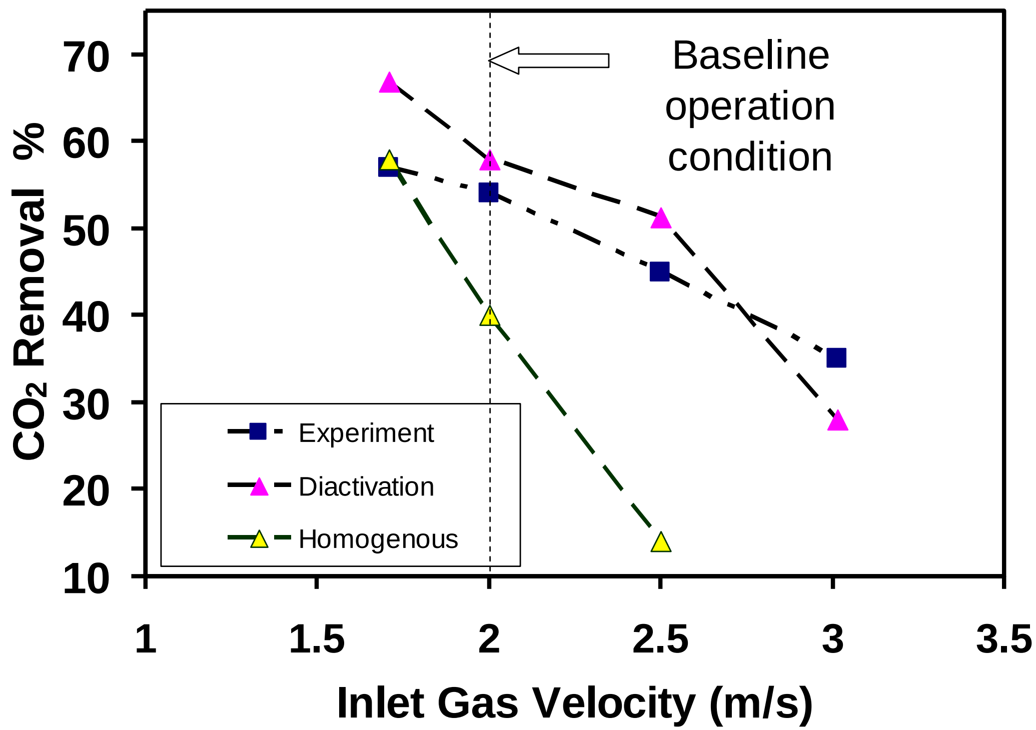
$$\%CO_2\ \text{removal} = \frac{X_{CO_{2,in}} - X_{CO_2}}{X_{CO_{2,in}}} \times 100\%$$



Contours of CO_2 mass fraction

Pressure Drop and Inlet Gas Velocity

	Time averaged Pressure drop (mm H2O) KIER Experiments	Time averaged Pressure drop (mm H2O) Simulation
DP1	100	107
DP2	200-500	335
DP3	250	270
DP4	70	73



Conclusion

- The simulation was able to capture the CO_2 removal percentage in line with experiment
- The calculated pressure drop is in good agreement with the experiment
- The simulation predicted cluster formation inside the riser using EMMS drag model

Moving Boundary Conditions

$$\frac{d\xi_{\min}}{dt} = \sum_{i=x,y,z} \left(-\frac{d\xi_{\min}}{dx_i} u_{p,i,\min} \right)$$

$$\frac{d\xi_{\max}}{dt} = \sum_{i=x,y,z} \left(-\frac{d\xi_{\max}}{dx_i} u_{p,i,\max} \right)$$

$$u_{p,i,\min}(t,x) = u_{p,i}(\xi = \xi_{\min}, t, x) = v_{p,i}(t,x) - \frac{D_{pt}(\xi = \xi_{\min}, t, x)}{f(\xi = \xi_{\min}, t, x)} [\frac{\partial f}{\partial x_i}(\xi = \xi_{\min}, t, x)]$$

$$u_{p,i,\max}(t,x) = u_{p,i}(\xi = \xi_{\max}, t, x) = v_{p,i}(t,x) - \frac{D_{pt}(\xi = \xi_{\max}, t, x)}{f(\xi = \xi_{\max}, t, x)} [\frac{\partial f}{\partial x_i}(\xi = \xi_{\max}, t, x)]$$

Moving Boundary Terms

$$MB = -\{[\overline{f'_{+1}} - (-1)^{i}.\overline{f'_{-1}}] - i.\mu_{i-1}\}.\frac{1}{(\xi_{\max} - \xi_{\min})}.(\frac{d\xi_{\min}}{dt} + \frac{d\xi_{\max}}{dt})$$
$$-\{[\overline{f'_{+1}} - (-1)^{i+1}.\overline{f'_{-1}}] - (i+1).\mu_{i}\}.\frac{1}{(\xi_{\max} - \xi_{\min})}.(-\frac{d\xi_{\min}}{dt} + \frac{d\xi_{\max}}{dt})$$

$$MB_{Conv} = -\{[\overline{f'_{+1}} - (-1)^{i}.\overline{f'_{-1}}] - i.\mu_{i-1}\}.\frac{v_{p,j}}{(\xi_{\max} - \xi_{\min})}.(\frac{\partial\xi_{\min}}{\partial x_j} + \frac{\partial\xi_{\max}}{\partial x_j})$$
$$-\{[\overline{f'_{+1}} - (-1)^{i+1}.\overline{f'_{-1}}] - (i+1).\mu_{i}\}.\frac{v_{p,j}}{(\xi_{\max} - \xi_{\min})}.(-\frac{\partial\xi_{\min}}{\partial x_j} + \frac{\partial\xi_{\max}}{\partial x_j})$$

Moving Boundary Terms

$$MB_{Diff\,1} = \frac{1}{(\xi_{\max}-\xi_{\min})}\left(\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j}\right)\int_{-1}^{+1}\frac{\partial D'_{pt}}{\partial x_j}\frac{\partial \overline{f'}}{\partial \bar{\xi}}(\bar{\xi})^i d\bar{\xi} +$$

$$\frac{1}{(\xi_{\max}-\xi_{\min})}\left(-\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j}\right)\int_{-1}^{+1}\frac{\partial D'_{pt}}{\partial x_j}\frac{\partial \overline{f'}}{\partial \bar{\xi}}(\bar{\xi})^{i+1} d\bar{\xi}$$

$$MB_{Diff\,3} = \frac{1}{(\xi_{\max}-\xi_{\min})}\left(\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j}\right)\int_{-1}^{+1}\frac{\partial D'_{pt}}{\partial \bar{\xi}}\frac{\partial \overline{f'}}{\partial x_j}(\bar{\xi})^i d\bar{\xi} +$$

$$\frac{1}{(\xi_{\max}-\xi_{\min})}\left(-\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j}\right)\int_{-1}^{+1}\frac{\partial D'_{pt}}{\partial \bar{\xi}}\frac{\partial \overline{f'}}{\partial x_j}(\bar{\xi})^{i+1} d\bar{\xi} -$$

$$\frac{1}{(\xi_{\max}-\xi_{\min})^2}\left[\left(\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j}\right)\right]^2\int_{-1}^{+1}\frac{\partial D'_{pt}}{\partial \bar{\xi}}\frac{\partial \overline{f'}}{\partial \bar{\xi}}(\bar{\xi})^i d\bar{\xi} -$$

$$\frac{1}{(\xi_{\max}-\xi_{\min})^2}.2.\left(\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j}\right)\left(-\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j}\right)\int_{-1}^{+1}\frac{\partial D'_{pt}}{\partial \bar{\xi}}\frac{\partial \overline{f'}}{\partial \bar{\xi}}(\bar{\xi})^{i+1} d\bar{\xi} -$$

$$\frac{1}{(\xi_{\max}-\xi_{\min})^2}\left(-\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j}\right)^2\int_{-1}^{+1}\frac{\partial D'_{pt}}{\partial \bar{\xi}}\frac{\partial \overline{f'}}{\partial \bar{\xi}}(\bar{\xi})^{i+2} d\bar{\xi}$$

Moving Boundary Terms

$$MB_{Diff\,2} = \frac{2}{(\xi_{\max}-\xi_{\min})}(\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j})\int_{-1}^{+1} D'_{pt}\frac{\partial^2 \overline{f'}}{\partial x_j \partial \overline{\xi}}(\overline{\xi})^i d\overline{\xi} +$$

$$\frac{2}{(\xi_{\max}-\xi_{\min})}(-\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j})\int_{-1}^{+1} D'_{pt}\frac{\partial^2 \overline{f'}}{\partial x_j \partial \overline{\xi}}(\overline{\xi})^{i+1} d\overline{\xi} -$$

$$\frac{1}{(\xi_{\max}-\xi_{\min})^2}[(\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j})]^2\int_{-1}^{+1} D'_{pt}\frac{\partial^2 \overline{f'}}{\partial \overline{\xi}^2}(\overline{\xi})^i d\overline{\xi} -$$

$$\frac{1}{(\xi_{\max}-\xi_{\min})^2}.2.(\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j})(-\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j})\int_{-1}^{+1} D'_{pt}\frac{\partial^2 \overline{f'}}{\partial \overline{\xi}^2}(\overline{\xi})^{i+1} d\overline{\xi} -$$

$$\frac{1}{(\xi_{\max}-\xi_{\min})^2}(-\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j})^2\int_{-1}^{+1} D'_{pt}\frac{\partial^2 \overline{f'}}{\partial \overline{\xi}^2}(\overline{\xi})^{i+2} d\overline{\xi} -$$

$$\frac{2}{(\xi_{\max}-\xi_{\min})^2}(-\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j})(\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j})\int_{-1}^{+1} D'_{pt}\frac{\partial \overline{f'}}{\partial \overline{\xi}}(\overline{\xi})^i d\overline{\xi} +$$

$$\frac{1}{(\xi_{\max}-\xi_{\min})}(\frac{\partial^2 \xi_{\min}}{\partial x_j{}^2}+\frac{\partial^2 \xi_{\max}}{\partial x_j{}^2})\int_{-1}^{+1} D'_{pt}\frac{\partial \overline{f'}}{\partial \overline{\xi}}(\overline{\xi})^i d\overline{\xi} -$$

$$\frac{1}{(\xi_{\max}-\xi_{\min})}.[(\frac{\partial^2 \xi_{\min}}{\partial x_j{}^2}-\frac{\partial^2 \xi_{\max}}{\partial x_j{}^2})+\frac{2}{(\xi_{\max}-\xi_{\min})}(-\frac{\partial \xi_{\min}}{\partial x_j}+\frac{\partial \xi_{\max}}{\partial x_j})^2]\int_{-1}^{+1} D'_{pt}\frac{\partial \overline{f'}}{\partial \overline{\xi}}(\overline{\xi})^{i+1} d\overline{\xi}$$