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Hamid Arastoopour
Illinois Institute of Technology, USA, arastoopour@iit.edu

WANGER INSTITUTE FOR SUSTAINABLE ENERGY RESEARCH

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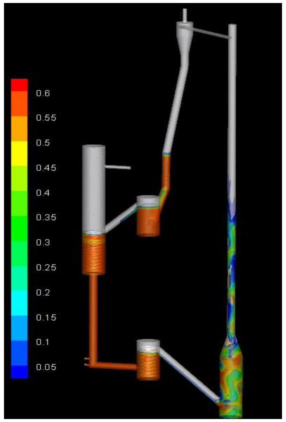
Three-Dimensional CFD Simulation of an MgO-based Sorbent Regeneration Reactor in a Carbon Capture Process

by

Emad Ghadirian, Javad Abbasian, and Hamid Arastoopour

Wanger Institute for Sustainable Energy Research (WISER)

Illinois Institute of Technology

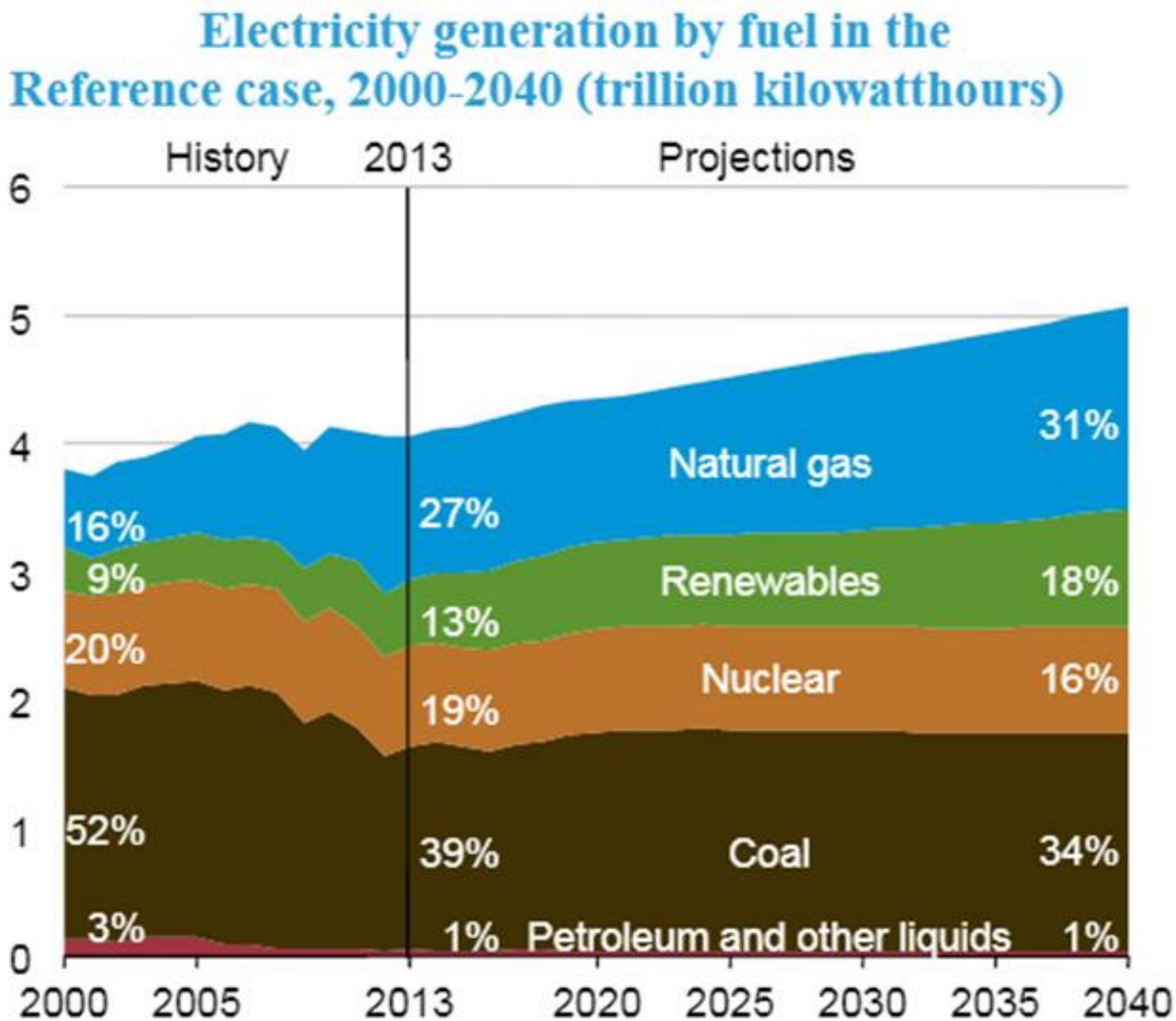


Fluidization XV, Engineering Conference International, Quebec, Canada May 2016

Outline

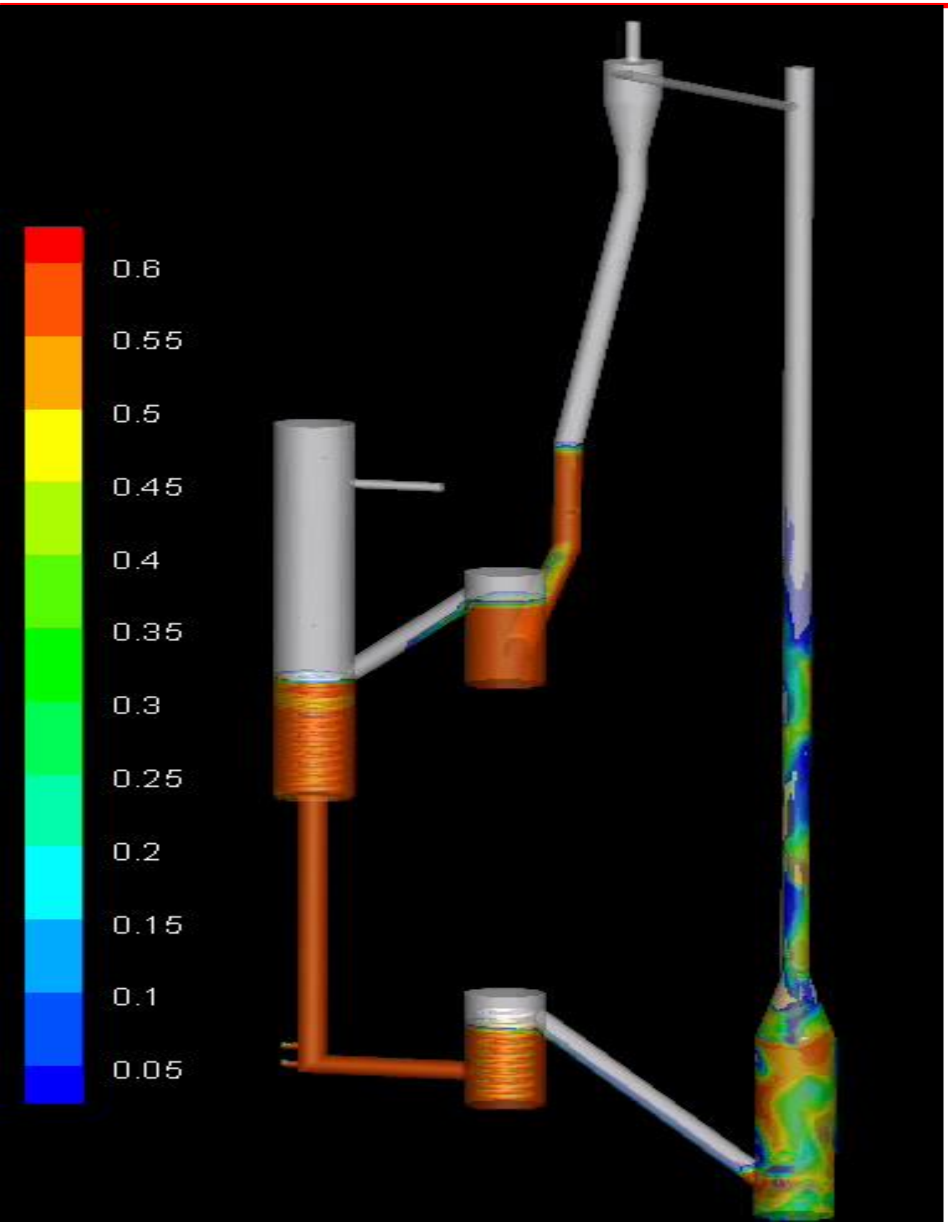
- Introduction
- Governing Two Fluid Model Equations
- Shrinking Core Model
- CFD Simulations and Case Studies
- Summary and Conclusion

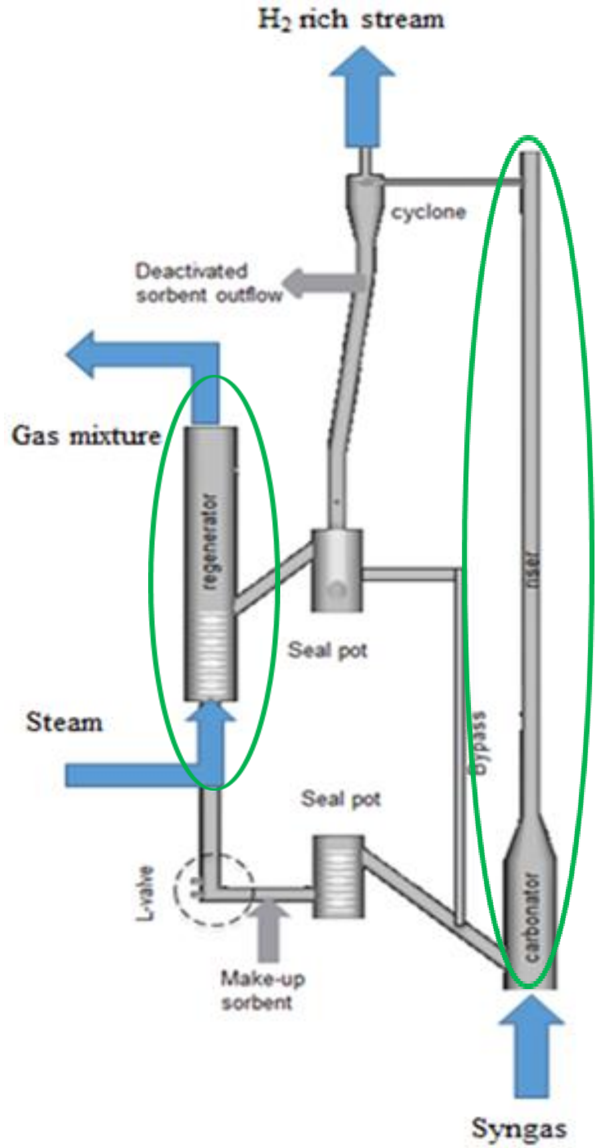
Motivation



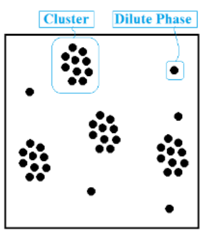
Source: "Annual Energy Outlook", EIA, 2015

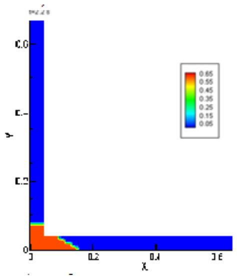
CO_2 Sorption (Carbonation) and CO_2 Regeneration Processes using a CFB System

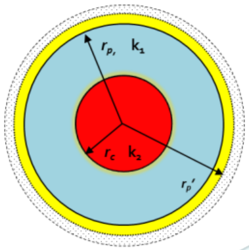


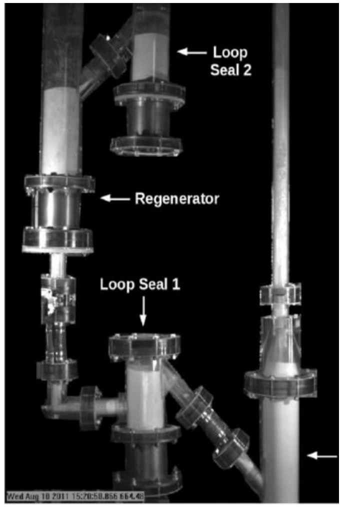


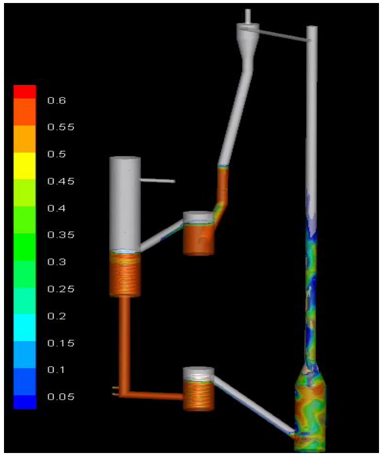
Project Roadmap

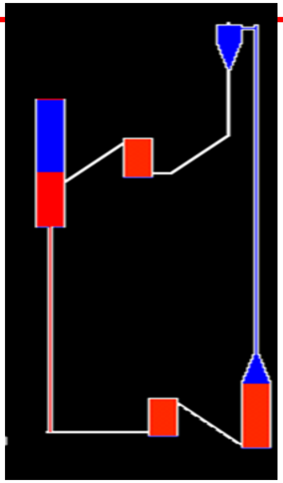












Sorbent Development

Fundamental

Studies and model development

Simulation and Validation

Bench Scale

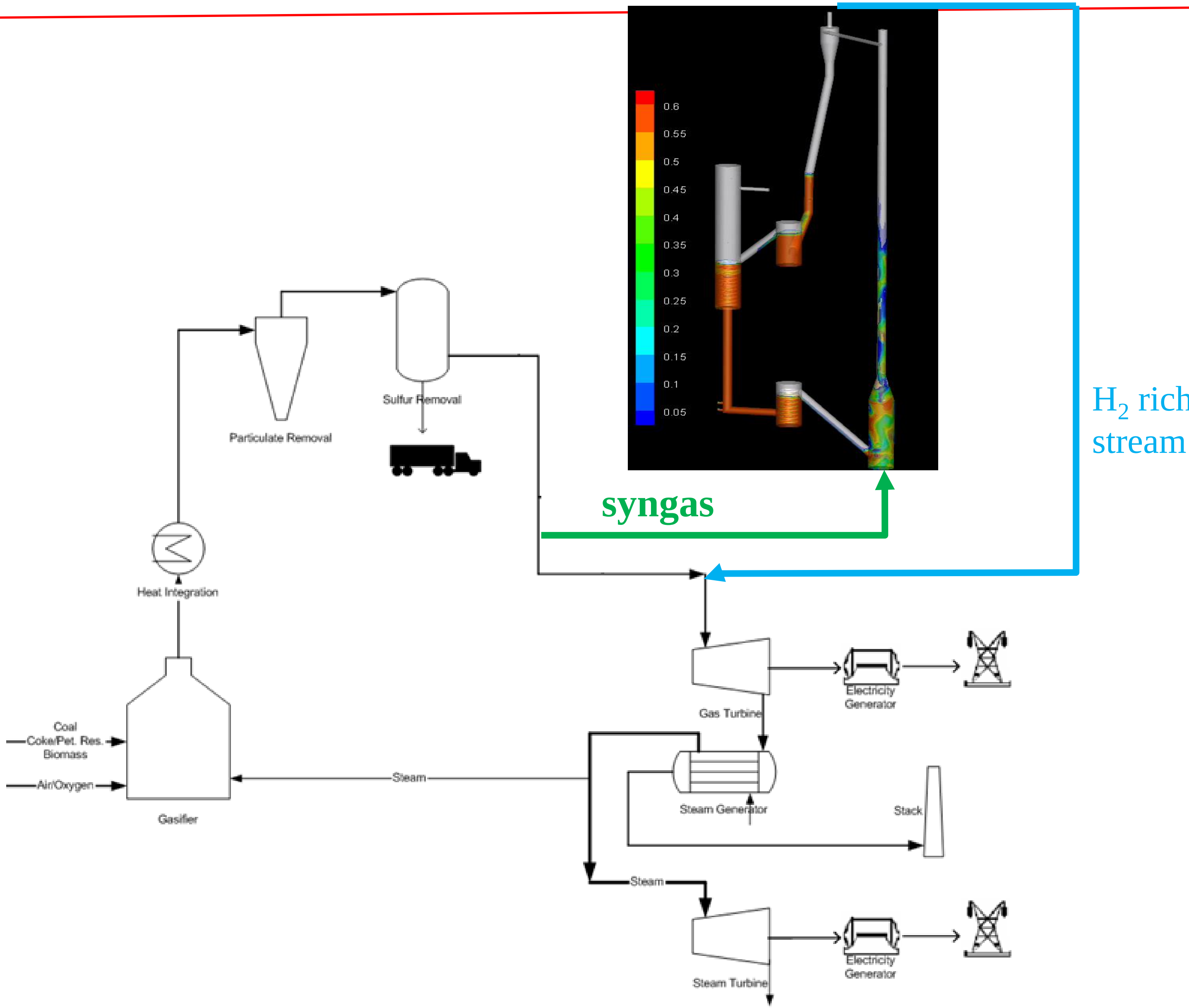
Low Pressure & Temperature

Cold CFB

High Pressure & Temperature

CFB reactor simulation

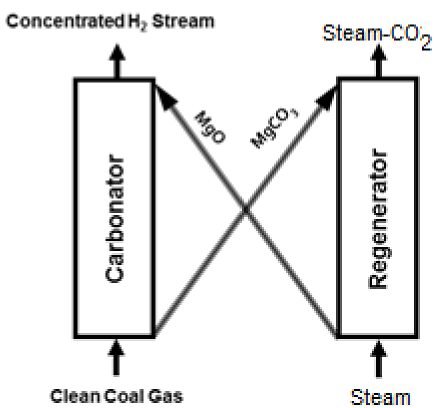
Schematic of IGCC Process

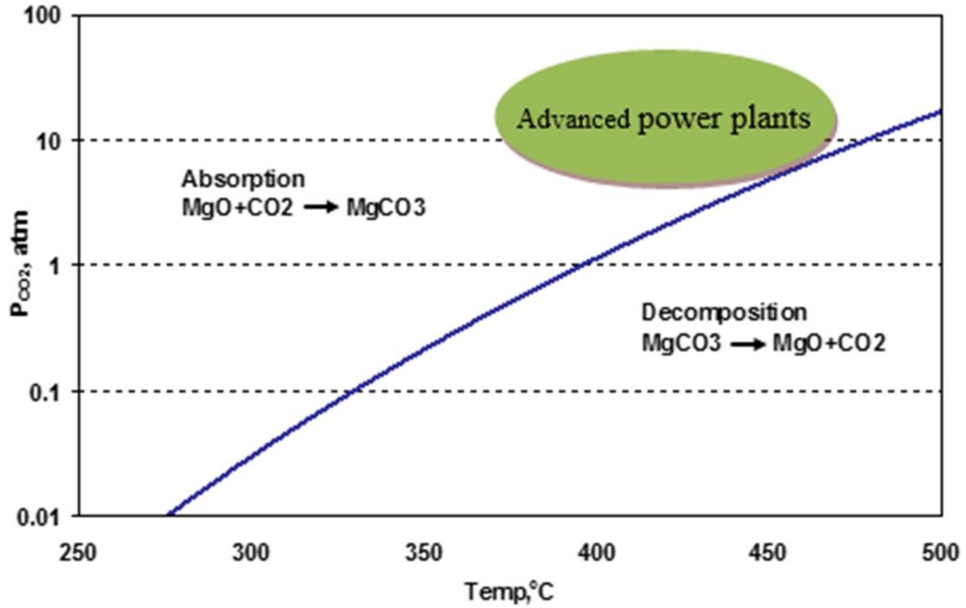


MgO-$MgCO_3$ Equilibrium

Process Economics is highly dependent on the CO_2 Sorbent properties

- **CO_2 absorption Temperature (300 - 450 ˚C)**
- **Simple regeneration**
- **Sulfur and Steam Resistant**
- **Sorbent Cost (per cycle)**





$$MgO + CO_2 \rightarrow MgCO_3$$

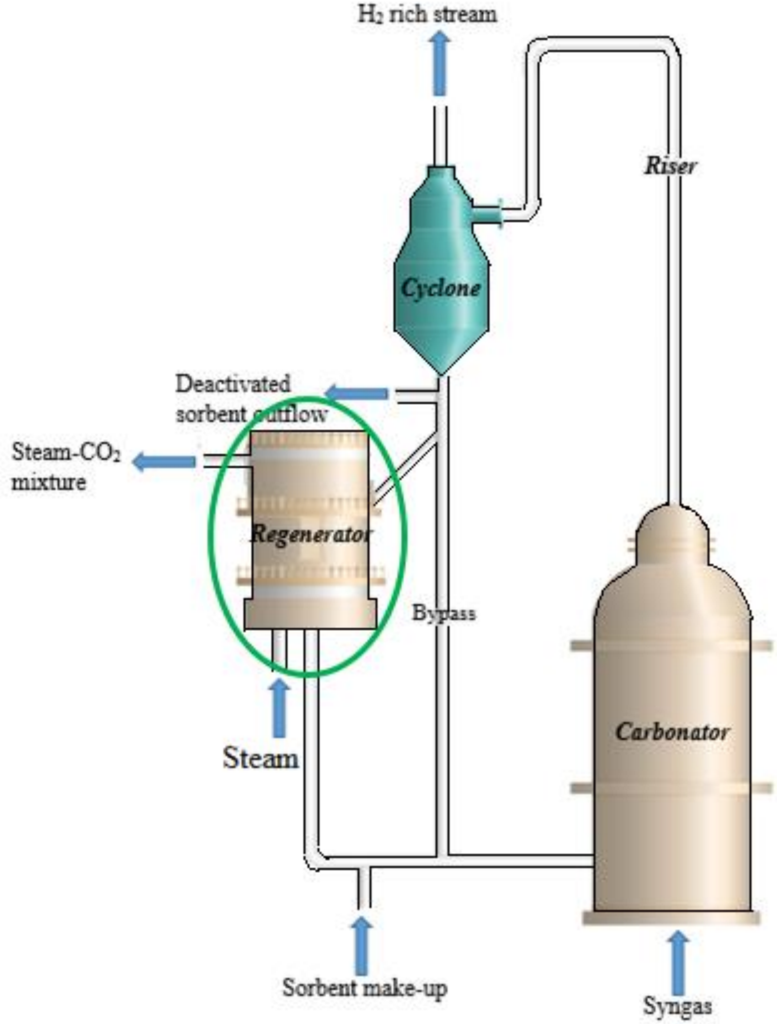
$$MgCO_3 \rightarrow MgO + CO_2$$

Objectives

- **To develop a numerical model for reactive gas-solid systems for the sorbent regeneration process at elevated temperature and pressure.**
- To achieve our objective:
  - Conducted experimental data on the regeneration reaction rate and used our data to develop an expression for rate of reaction and incorporated it in our CFD model
  - Developed and incorporated appropriate constitutive equations in our CFD model

Specific objective of this study

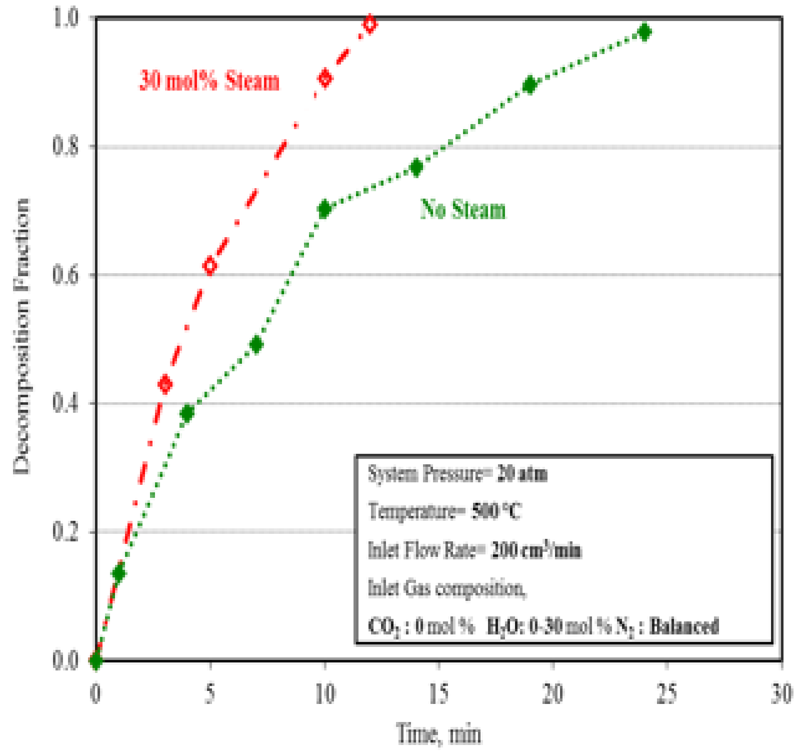
- Conducted Simulations for CO_2 regeneration of Carbonated MgO-Based Solid Sorbent using ANSYS FLUENT computer code



Experimental Data on Sorbent Regeneration

$$MgCO_3 \rightarrow MgO + CO_2$$

Effect of steam on Sorbent Regenerability

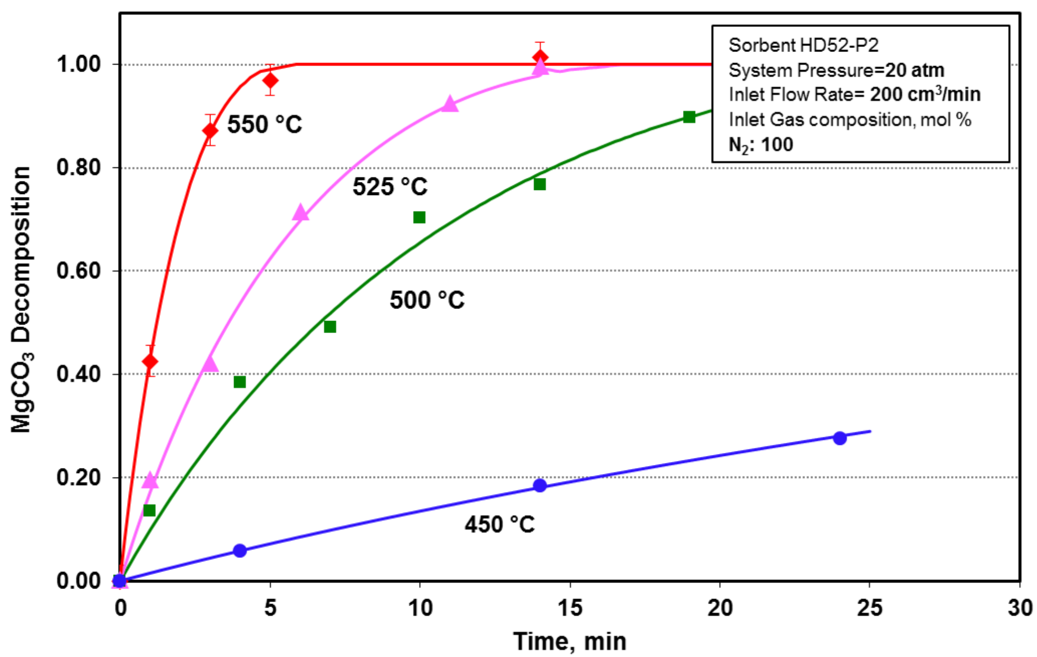


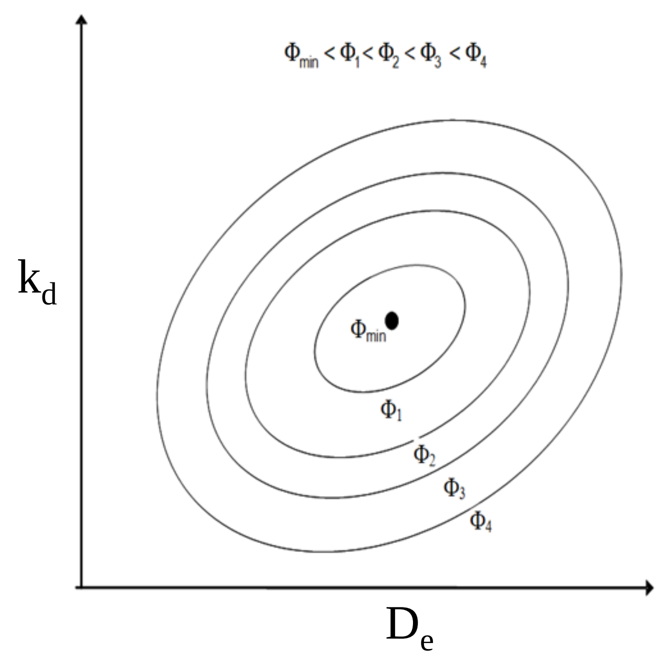
Shrinking Core Model Fit

$$MgCO_3 \rightarrow MgO + CO_2$$

$$\frac{dx}{dt} = \frac{3}{r_p}\frac{k_d}{N^0_{MgCO_3}}(1-x)^{1/3}\left(1-\frac{C_i}{C_e}\right)^2$$

$$C_i = \frac{k_d R_g T r_p (1-x)^{1/3}}{D_e}\left(1-\frac{C_i}{C_e}\right)^2\left[(1-x)^{1/3}-1\right] + C_b$$





Governing Equations

Conservation of mass:

$$\frac{\partial(\alpha_g \rho_g)}{\partial t} + \nabla.\left(\alpha_g \rho_g \vec{v}\right) = \dot{m}_g$$

$$\frac{\partial(\alpha_p \rho_p)}{\partial t} + \nabla.\left(\alpha_p \rho_p \vec{v}\right) = \dot{m}_p = -\dot{m}_g$$

Conservation of momentum:

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g \vec{v}_g\right) + \nabla.\left(\alpha_g \rho_g \vec{v}_g \vec{v}_g\right) = -\alpha_g \nabla P + \nabla.\bar{\bar{\tau}}_g + \alpha_g \rho_g \vec{g} - \bar{\beta}\left(\vec{v}_g - \vec{v}_s\right)$$

$$\frac{\partial}{\partial t}\left(\alpha_p \rho_p \vec{v}_p\right) + \nabla.\left(\alpha_p \rho_p \vec{v}_p \vec{v}_p\right) = -\alpha_p \nabla P - \nabla P_p + \nabla.\bar{\bar{\tau}}_p + \alpha_p \rho_p \vec{g} + \bar{\beta}\left(\vec{v}_g - \vec{v}_p\right)$$

Conservation of particulate phase fluctuating energy:

$$\frac{3}{2}\left(\frac{\partial}{\partial t}\left(\rho_p \alpha_p \theta_p\right) + \nabla.\left(\rho_p \alpha_p \vec{v}_p \theta_p\right)\right) = \left(-P_p \bar{\bar{I}} + \bar{\bar{\tau}}_p\right):\nabla \vec{v}_p + \nabla.\left(k_{\theta_p} \nabla \theta_p\right) - \gamma_p$$

Governing Equations

$$MgCO_3 \rightarrow MgO + CO_2$$

Conservation of species:

$$\frac{\partial}{\partial t}\left(\alpha_p \rho_p y_{ip}\right) + \nabla.\left(\alpha_p \rho_p v_p y_{ip}\right) = R_i = \frac{1}{MW_{MgCO_3}} N^0_{MgCO_3} \frac{dx}{dt}$$

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g y_{jg}\right) + \nabla.\left(\alpha_g \rho_g v_g y_{jg}\right) = -R_i \qquad j = CO_2, i = MgO, MgCO_3$$

Regeneration (Shrinking core model-2nd order)

$$\frac{dx}{dt} = \frac{3}{r_p} \frac{k_d}{N^0_{MgCO_3}} (1-x)^{1/3} \left(1 - \frac{C_i}{C_e}\right)^2$$

$$C_i = \frac{k_d R_g T r_p (1-x)^{1/3}}{D_e} \left(1 - \frac{C_i}{C_e}\right)^2 \left[(1-x)^{1/3} - 1\right] + C_b$$

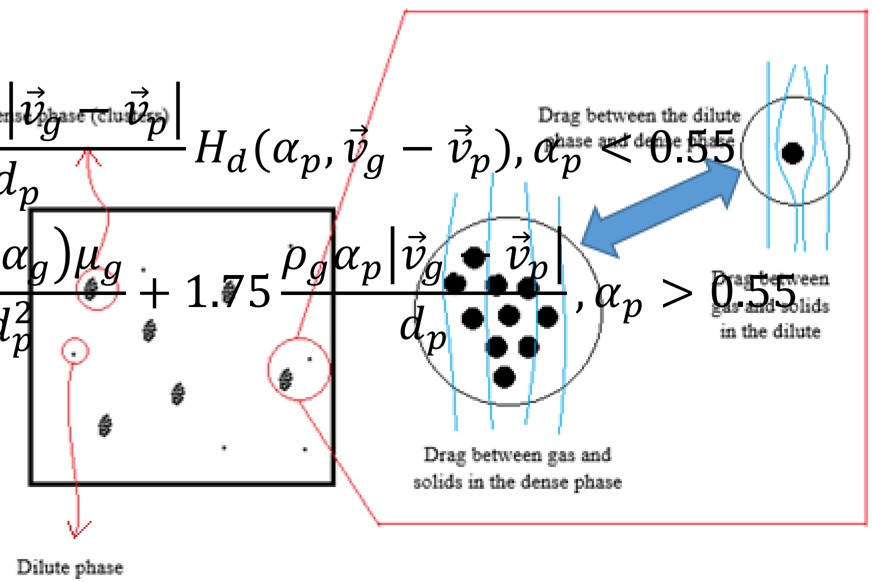
Drag Force

Non-homogeneous dispersion of particulate phase in the gas phase: Energy Minimization Multi-Scale (EMMS)

- Considers the presence and distribution of clusters
- Considers the effect of clusters on drag force reduction in fluidized beds
- Is based on minimization of total energy for suspending and transporting the particles

$$\bar{\beta} = \begin{cases} \frac{3}{4} C_d \frac{\alpha_p \alpha_g \rho_g |\vec{v}_g - \vec{v}_p|}{d_p} H_d(\alpha_p, \vec{v}_g - \vec{v}_p), \alpha_p < 0.55 \\ 150 \frac{\alpha_p (1 - \alpha_g) \mu_g}{\alpha_g d_p^2} + 1.75 \frac{\rho_g \alpha_p |\vec{v}_g - \vec{v}_p|}{d_p}, \alpha_p > 0.55 \end{cases}$$

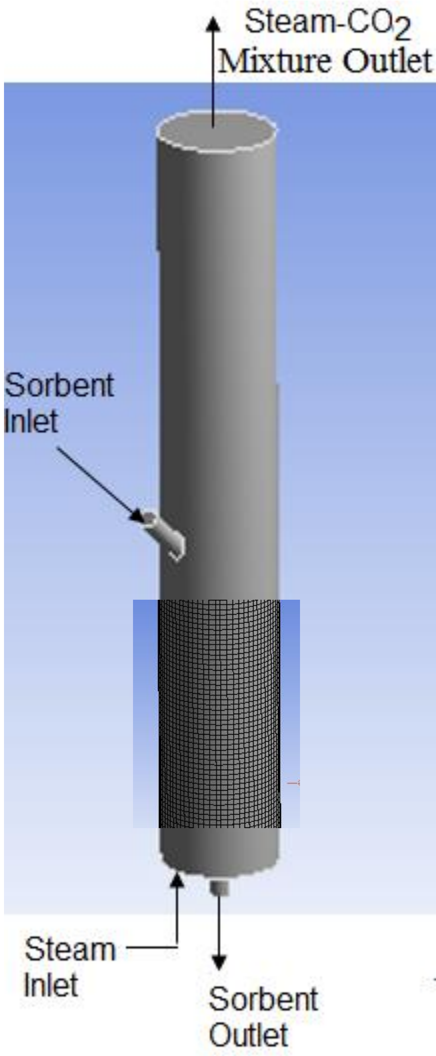
$$H_d = \frac{F_{EMMS}}{F_{Wen\,\&\,Yu}}$$



3D Simulation of Regenerator

$$MgCO_3 \rightarrow MgO + CO_2$$

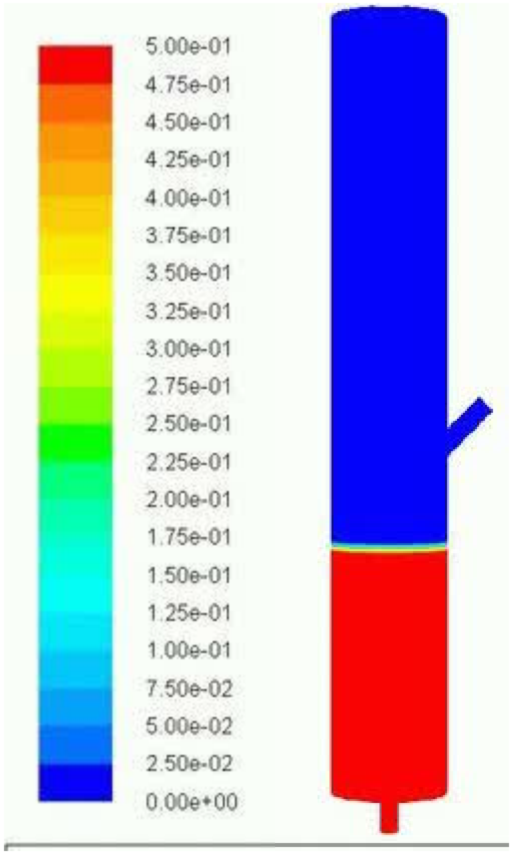
	Base Case	Case Study 1	Case Study 2	Case Study 3
Temperature	500 C	500 C	500 C	500 C
Pressure	50 atm	20 atm	50 atm	50 atm
Solid rate	24 g/s	24 g/s	120 g/s	24 g/s
Steam inlet velocity	0.075 m/s	0.075 m/s	0.075 m/s	0.15 m/s



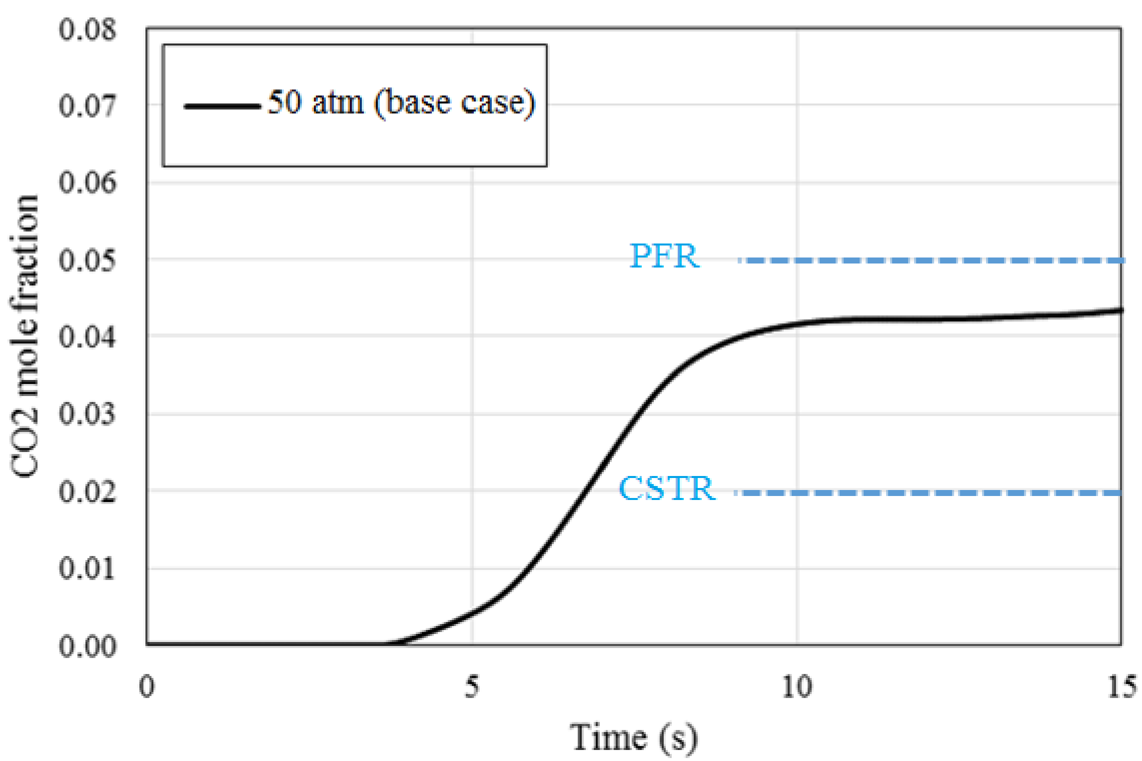
Simulation of Regenerator

$$MgCO_3 \rightarrow MgO + CO_2$$

Solid volume fraction



CO_2 mole fraction

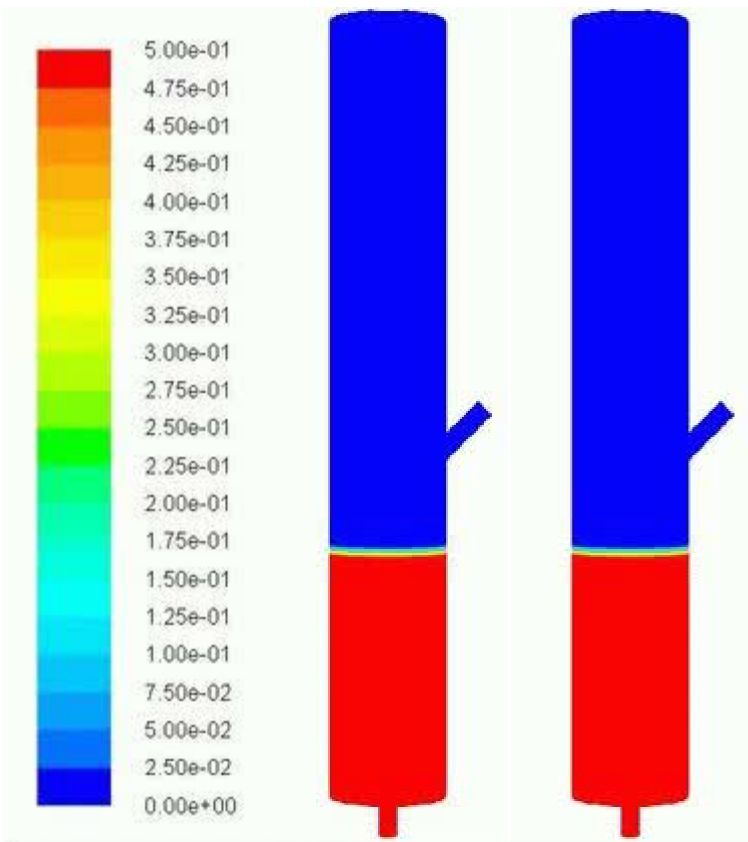


Effect of Pressure on CO_2 Regeneration

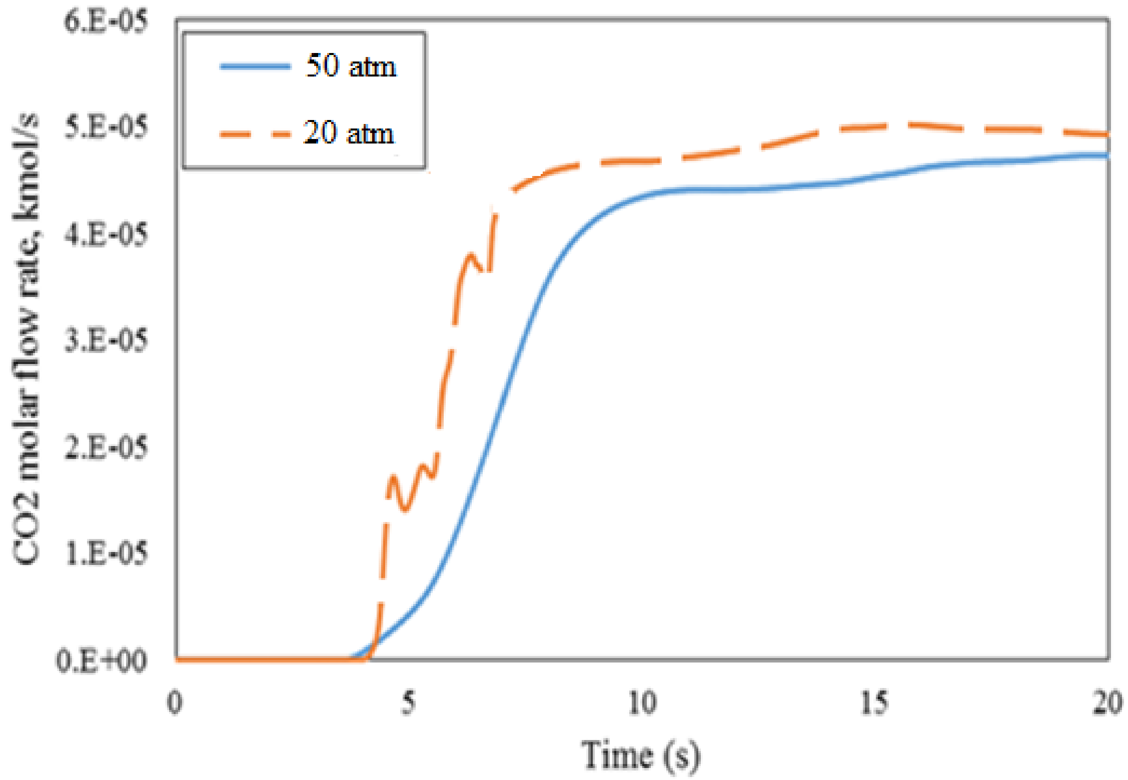
$$MgCO_3 \rightarrow MgO + CO_2$$

Solid volume fraction

CO_2 molar flow rate

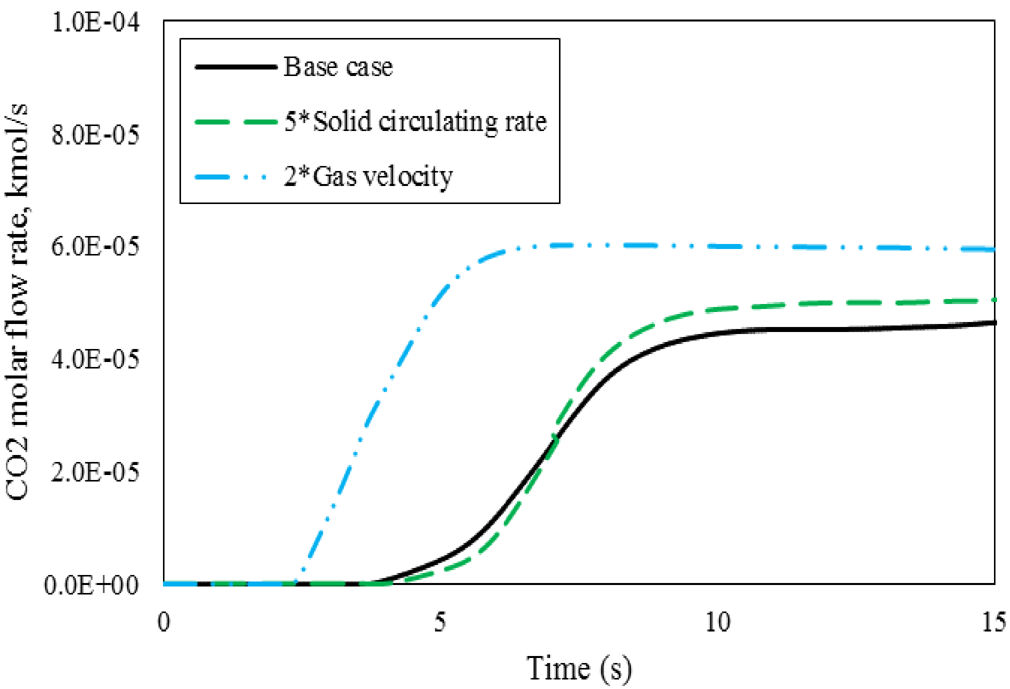


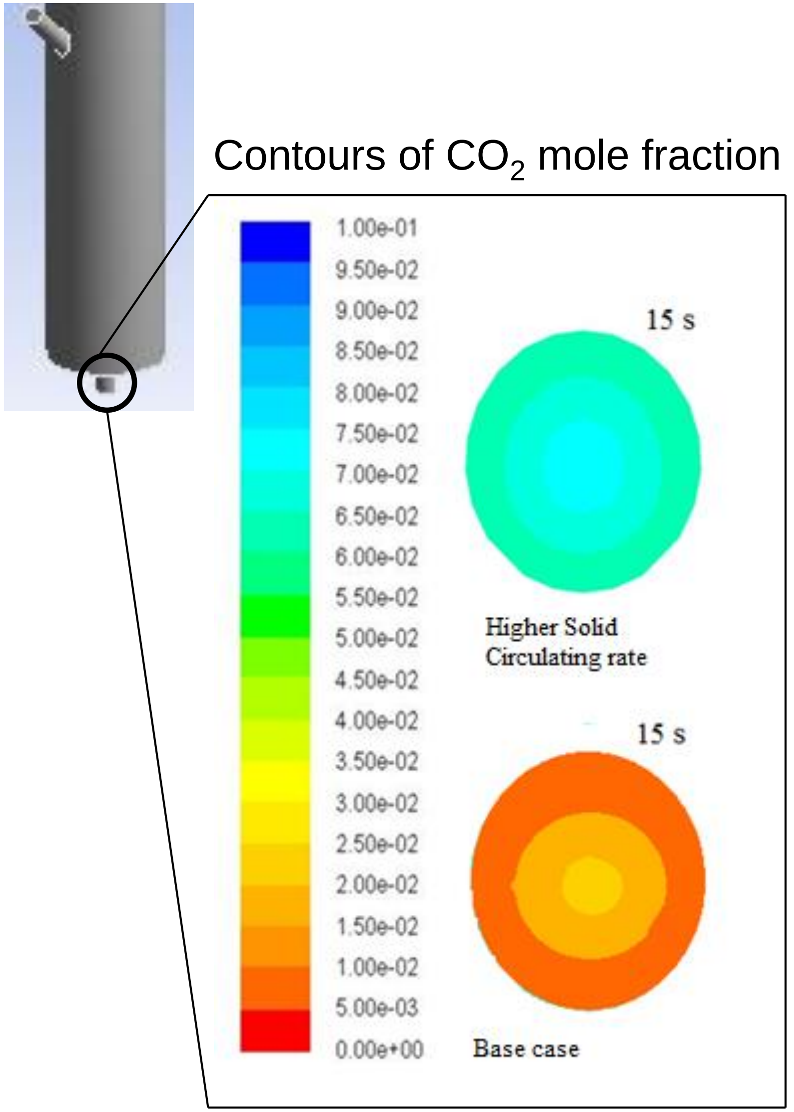
50 atm 20 atm



Effect of Gas and Solid Flowrates

$$MgCO_3 \rightarrow MgO + CO_2$$





Summary and Conclusion

- Computational Fluid Dynamics (CFD) along with drag expression based on EMMS approach and Shrinking core model described well CO_2 regeneration process using MgO-based sorbents.
- Our simulation showed that operating the regenerator at high pressures (e.g. 50 atm) allowed us to use higher gas velocity and solid circulating rate without back-mixing of the solids which occurred at moderate pressures.
- Higher steam velocity in the system was shown to dilute the system with regard to CO_2 mole fraction and resulted in an improvement in sorbent regeneration.
- Higher solid circulating rate was shown to increase the amount of CO_2 leaving the system from the bottom of the reactor with regenerated sorbents.