CFD modeling and simulation for sorbent based CO_2 capture systems

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U.S. DEPARTMENT OF ENERGY

Outline

Team

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I. Sorbent Based CO_2 Capture
II. KIER Dual Fluidized-bed Reactor
III. Sub-models
IV. Results
V. Conclusions

CO_2 Capture Ready Fossil Energy

- Address concerns over increased CO_2 concentration leading to climate change

- Challenge:
  - provide cost effective options to reduce CO2 emissions
  - meet growing energy demands
  - coal
    - large supply
    - Also address existing production capacity

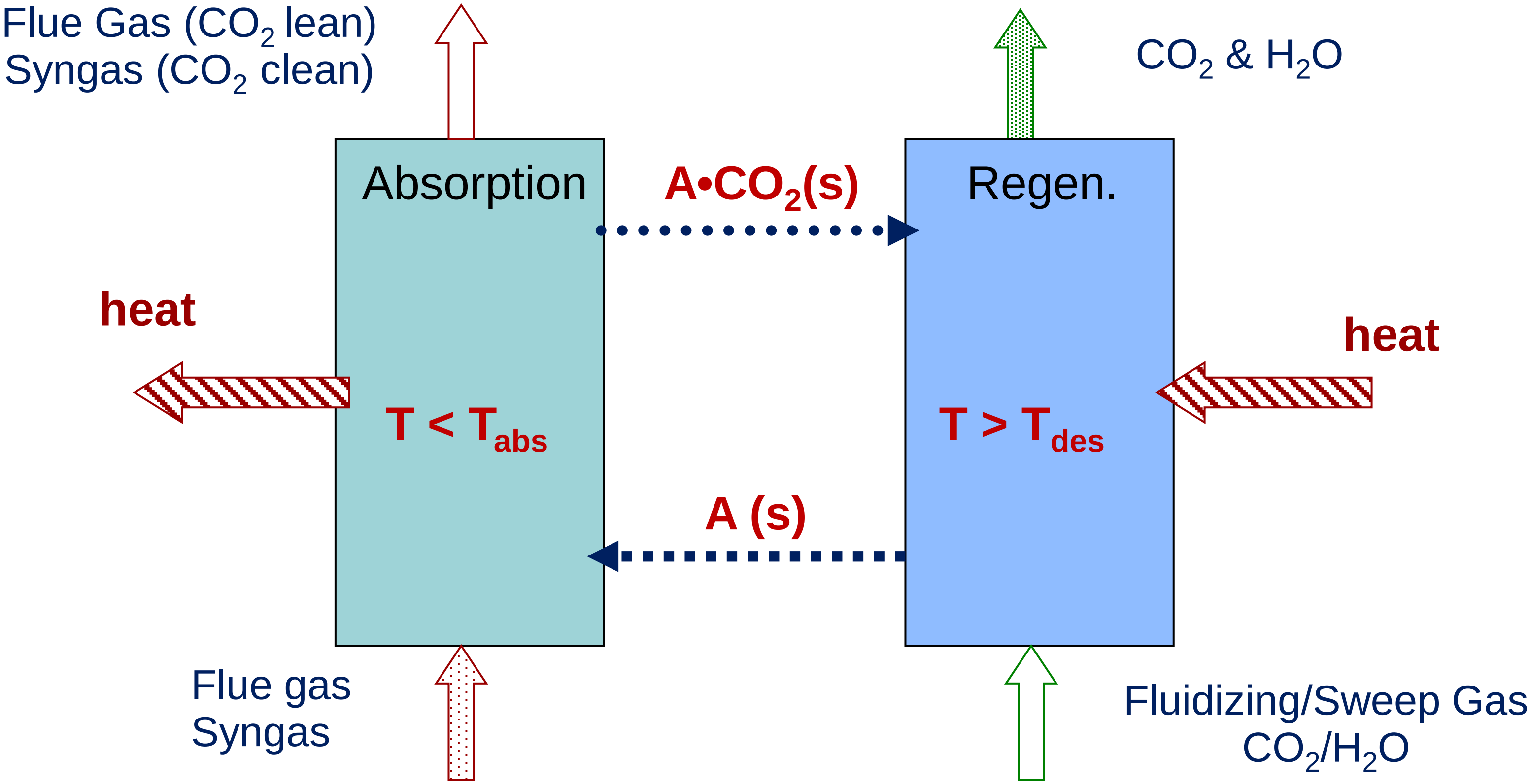
- Candidates systems [Wall 2007]:
  - oxyfuel combustion (including fluidized bed)
  - chemical looping
    - combustion, gasification, uncoupling, reforming,…
  - pre-combustion CO_2 separation (gasification)
  - ***post-combustion CO_2 separation***

Post-Combustion Capture

- **Commercially available systems**
  - amine liquid solvent system
  - significant energy penalty

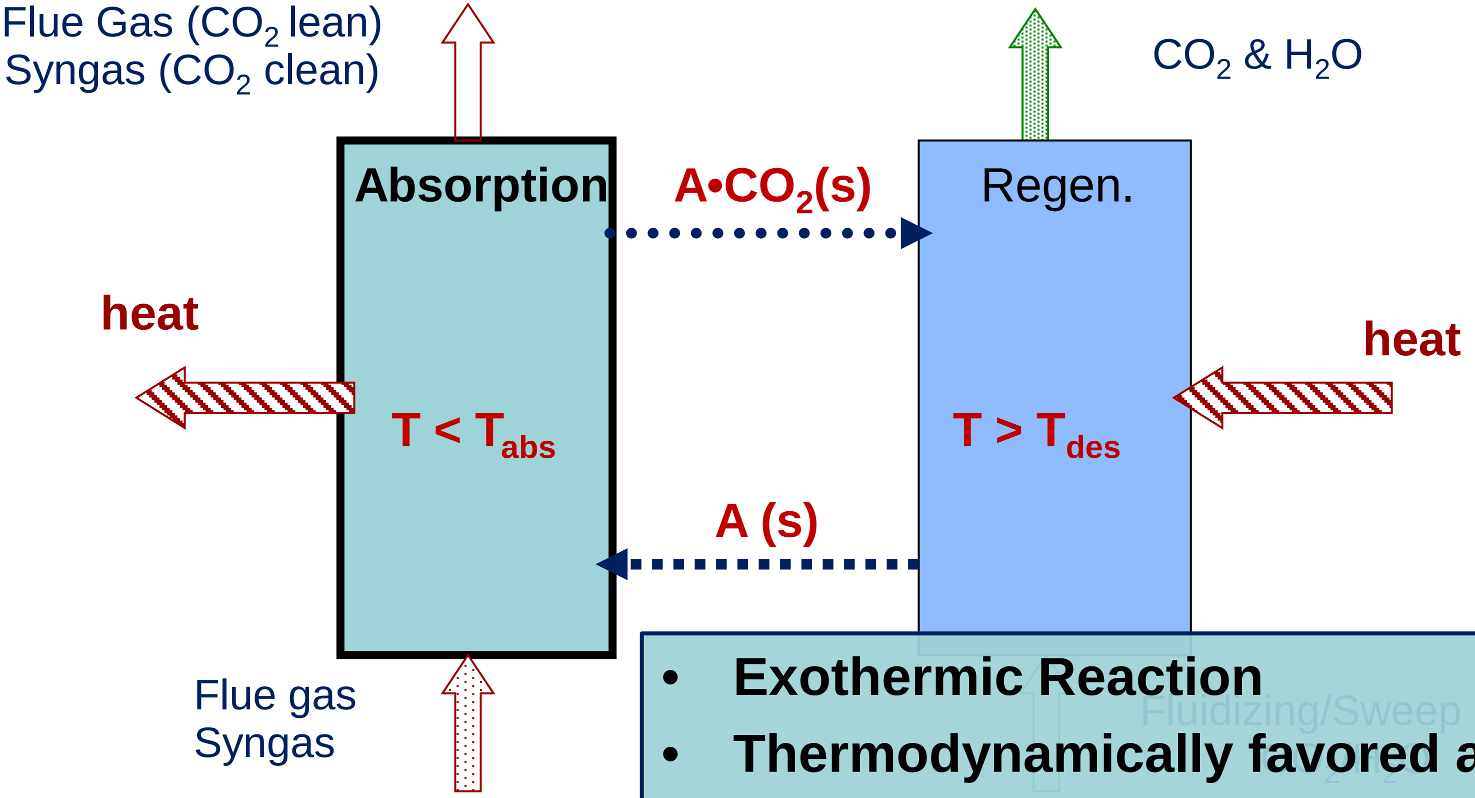
- **Research Areas**
  - ***solid-sorbents***
  - algaes
  - membranes
  - low-energy solvent processes
  - encapsulated solvents
  - …..

Sorbent-based CO_2 Capture



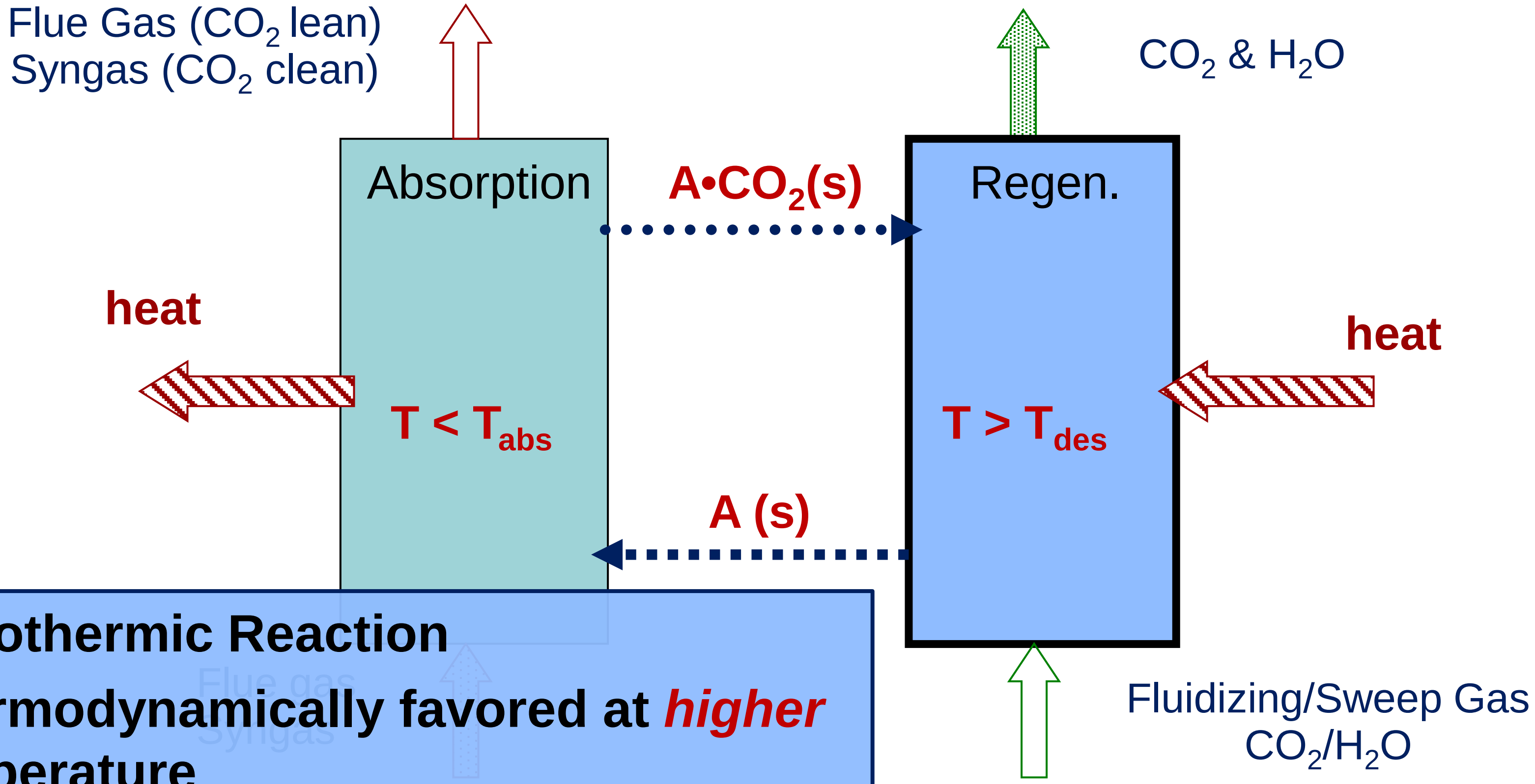
- **Dual reactor system for removing CO2 from flue or syngas**

CO_2 Capture



- **Exothermic Reaction**
- **Thermodynamically favored at *lower* temperature**
  - Must remove heat to prevent desorption and reduce solids temperature

Regeneration



- **Endothermic Reaction**
- **Thermodynamically favored at *higher* temperature**
  - Add heat to increase particle temperature and to sustain process

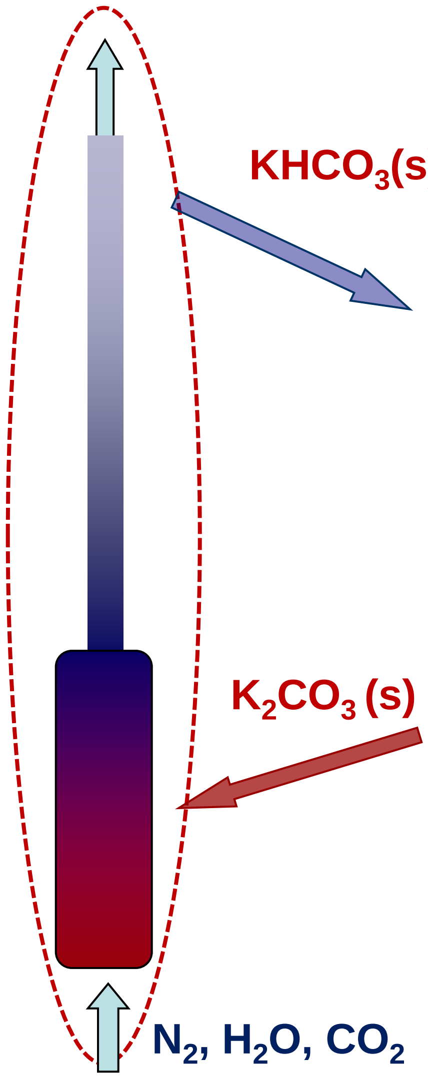
Technical Challenges

- **Technical Challenges**
  - Heat management
  - Water condensation
  - Carrier capacity, reactivity, sensitivity to sweep gas

- **CFD Modeling**
  - Help identify requirements for sorbent design (kinetics, attrition, capacity)
  - Reactor Scale-up
  - …..

KIER Carbonator/Regenerator

Yi, Jo, Seo, Lee, Ryu (2007)



CO_2 & H_2O
depleted gas

KHCO$_3$(s)

H_2O, CO_2, N_2

Riser
5.4 m x 25 mm
T ≈ 330-360 K

Bubbling Bed
1.2 m x 100 mm
T ≈ 390-490 K

$2KHCO_3$ (+ heat) →
$K_2CO_3 + CO_2 + H_2O$

K_2CO_3(s)

Fast Fluidized Bed
0.6 m x 35 mm
T ≈ 330-360 K

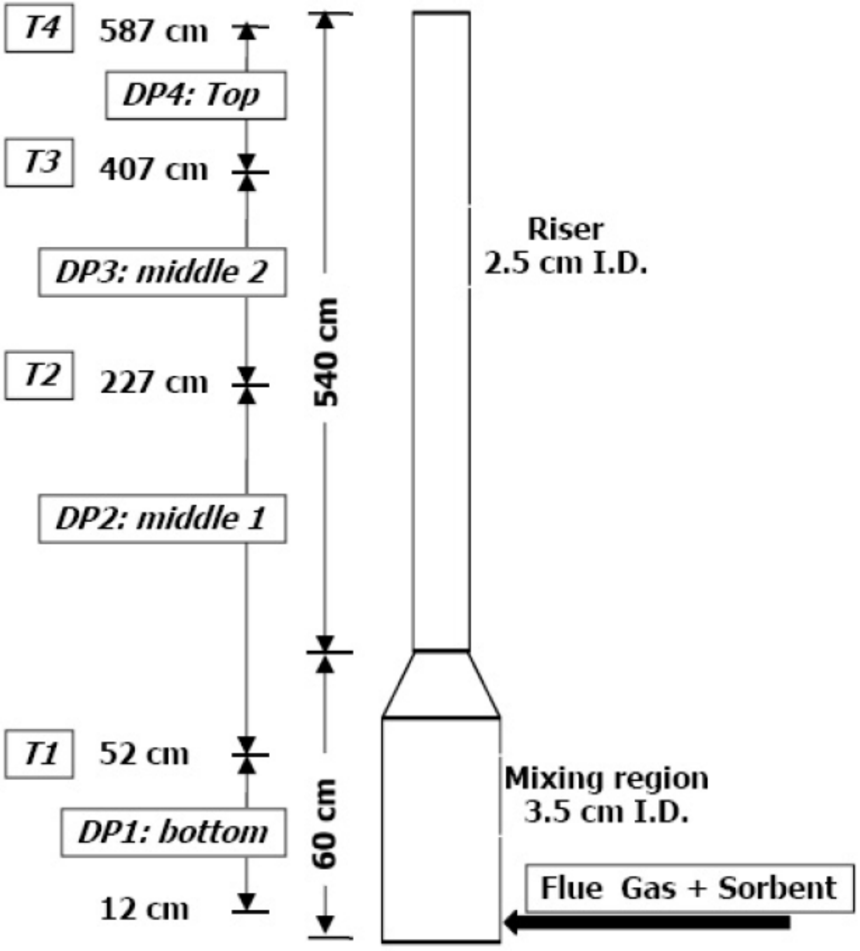
H_2O, N_2

$K_2CO_3 + CO_2 + H_2O$
→ $2KHCO_3$ (+ heat)

N_2, H_2O, CO_2

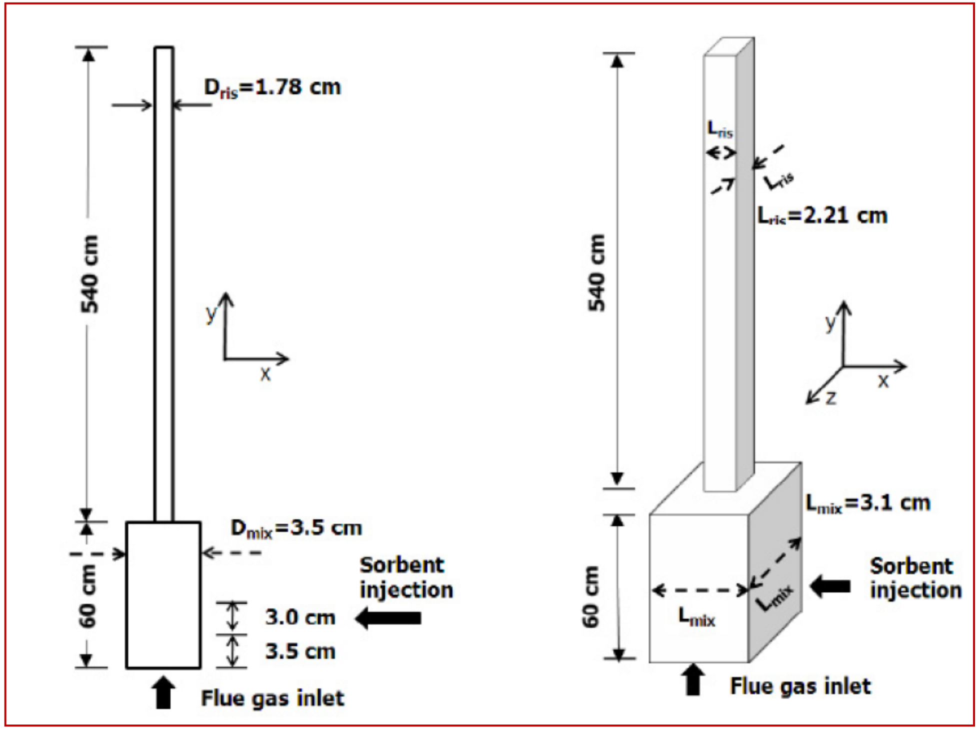
Absorber Operating Conditions

Gas	
Pressure	1 atm
Inlet Temperature	350 K
Mass Flow Rate	1 g/s & variable
wt% N2:H2O:CO2	75, 10, 15
Sorbent	
Inlet Temperature	350 K
Circulation Rate	10 g/s & variable
wt% C:K2CO3:KHCO3	65, 0, 35
Density	1.1 g/cm3
Diameter	100 μm



MFIX Model

- **Rectangular Geometry**
    - Cartesian mesh for MFIX
    - Match area as opposed to width
- “Model A”
- **Discretization**
    - Backward Euler
    - Momentum superbee
    - Remainder upwind



	$\Delta x \bullet \Delta y \bullet \Delta z$ (cm)
2D	0.206 x 1.0
2D fine	0.103 x 0.5
3D	0.206 x 1.0 x 0.206

Chemical Reaction Model

- **Homogeneous Reaction Model**

  (Park et al., J. Ind. Eng. Chem, 2006)

$$\frac{d}{dt}\left(\varepsilon_s \rho_s X_{K_2CO_3}\right) = -\varepsilon_s k_1 \left[K_2CO_3\right]\left[CO_2\right]$$

Form used for most simulations

$$\frac{d}{dt}\left(\varepsilon_s \rho_s X_{K_2CO_3}\right) = -\varepsilon_s k_2 \left[K_2CO_3\right]\left[CO_2\right]\left[H_2O\right]$$

- **Calculate constants to roughly match CO_2 capture**
  - k_1= 500 cm^3/mol/s, k_2= 6 x 10^7 cm^6/mol^2/s
- **Neglects**
  - Transport resistances (external/internal)
  - Rate increase due to temperature
  - Reverse rate

Drag Model

- **Gidaspow (Ergun/Wen-Yu) & EMMS**

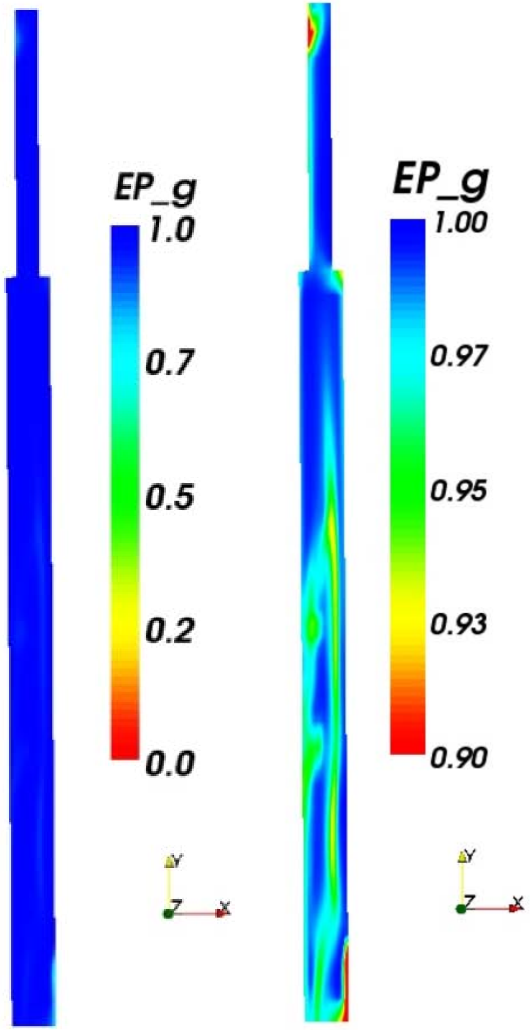
$$\beta = \begin{cases} \frac{3}{4} C_D \frac{\rho_g \varepsilon_g \varepsilon_s \left|\mathbf{U}_g - \mathbf{U}_s\right|}{D_p} \boxed{\varepsilon_g^{-2.65} H(\varepsilon_g, \mathrm{Re})}, \\ 150 \frac{\varepsilon_s (1-\varepsilon_g) \mu_g}{\varepsilon_g {D_p}^2} + 1.75 \frac{\rho_g}{{D_p}^2} \varepsilon_s \left|\mathbf{U}_g - \mathbf{U}_s\right|, \end{cases} \tag{15}$$

- **H, heterogeneity index**
  - Use curve fits from Lu et. al. [2009]
  - Differences in solids properties and flow conditions

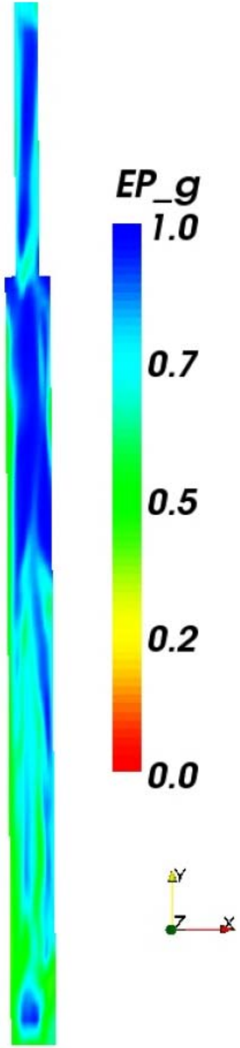
	Lu et. al.	KIER
ρ_p (kg/m^3)	930	1100
U_g (m/s)	1.5	1-3
G_s (kg/m^2/s)	50-160	10-30
d_p (µm)	54	100

Lu, Wang, Lia, 2009, - Chem. Eng Sci. (64) pp. 3437 -- 3447

Voidage Contours



Gidaspow

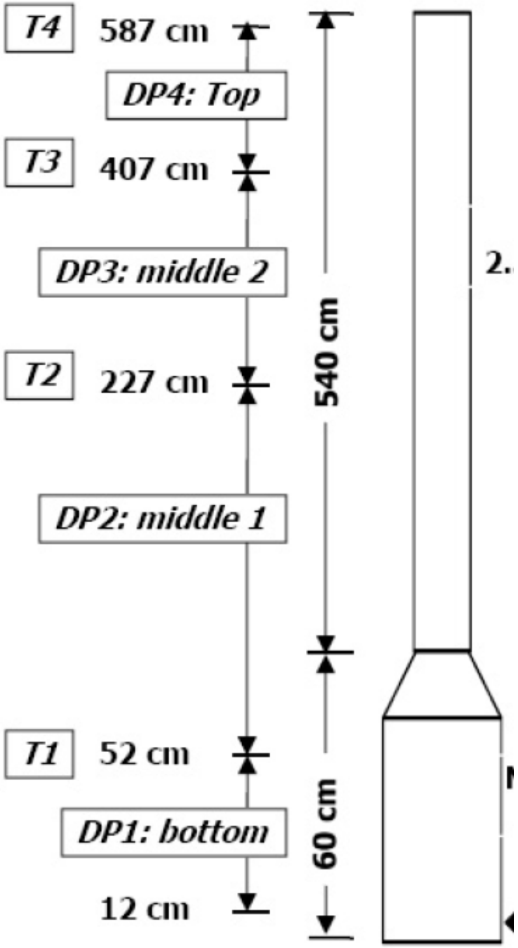


EMMS

Note color scale

- **Simulations using EMMS drag model predict more solids inventory**

Pressure Drop

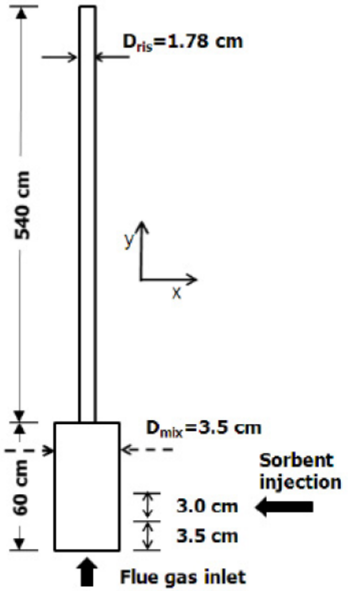


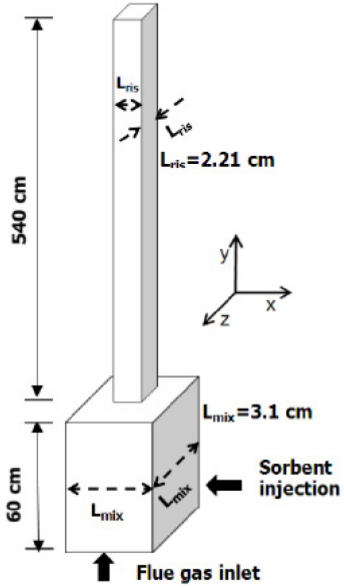
- Pressure drop prediction are closer to experiments with EMMS drag

Pressure difference (mm H_2O)	EMMS coarse	EMMS fine	Gidaspow coarse	Yi et al. (2007)
DP1	80	103	10	100-190
DP2	239	250	28	200-500
DP3	205	226	26	200
DP4	170	176	25	70

2D vs. 3D Results

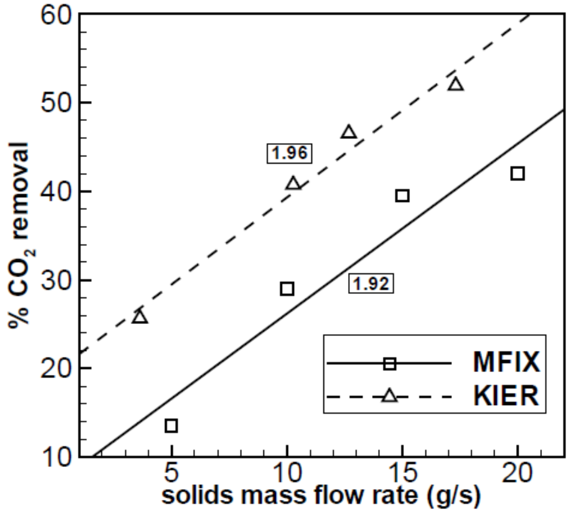
Pressure difference (mm H_2O)	2D 15 g/s	3D 15 g/s	Yi et al.(2007)
DP1	80	140	100-190
DP2	230	291	200-500
DP3	205	229	200
DP4	170	121	70

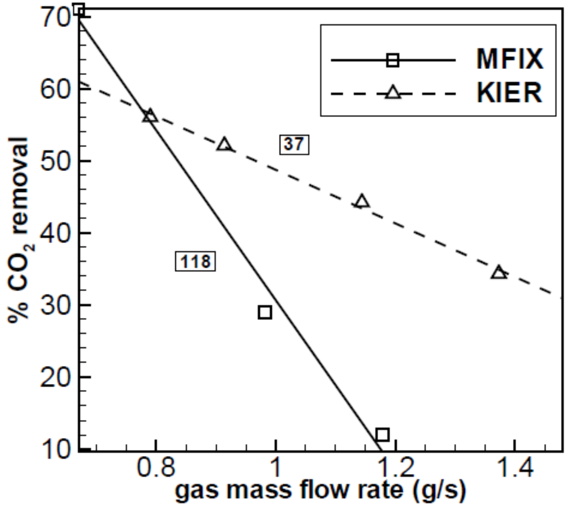




- **Similar differential pressure predictions, but..**
  - 2D - 4 processor for 4 days → 16 CPU-days
  - 3D - 16 processors for 34 days → 544 CPU-days

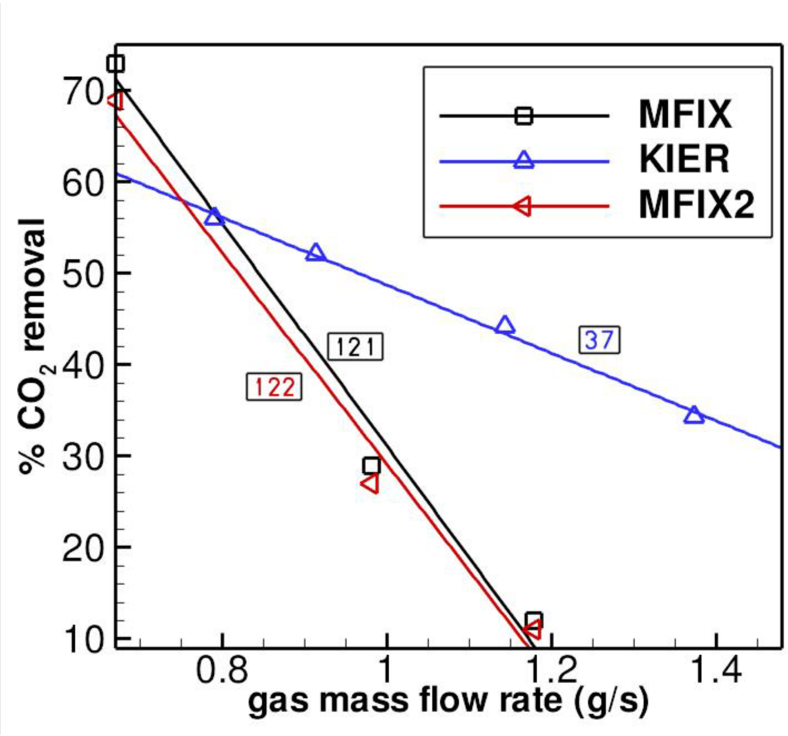
CO$_2$ Removal





- **Similar** sensitivity to the *solids flow rate* as experiment
- **Over-prediction** of the sensitivity to the *gas flow rate.* ***Why ?***
  - – reaction model
    - *water vapor concentration*
    - *transport resistances*
  - – drag model
    - *operating regime*
    - *particle properties*
  - – Numerics/setup

Effect of Reaction Model



- Inclusion of the *water vapor concentration* term in the reaction rate does not significantly change model sensitivity to the *gas flow rate*

$$(MFIX) \quad RR_1 = -\varepsilon_s k_1 [K_2CO_3][CO_2]$$

$$(MFIX1) \quad RR_2 = -\varepsilon_s k_2 [K_2CO_3][CO_2][H_2O]$$

Future Work

- **Drag Model**
  - EMMS drag for sorbent and operating regime
  - explore other cluster corrections
- **Reaction Model** – include neglected processes
  - transport resistances
  - reaction rate increase with temperature
  - reverse reaction
- **Model refinements**
  - resolution
  - geometric representation (cut-cell, cylindrical)
  - approaches (Eulerian-Lagrangian)
- **KIER Regenerator & Other Systems**

Conclusions

- **Performed MFIX simulations of KIER CO_2 absorption reactor**
  - Predict sensitivity of capture with respect to solids flow rate within 2% of measurements.
  - Over-predict (~ 3X) sensitivity of capture with respect to gas flow rate.
- **Drag model which accounts for non-homogenous solid distribution seem to be more important than**
  - resolution
  - geometrical details