GPU-based algorithm for numerical simulation of CO_2 sorption

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Introduction

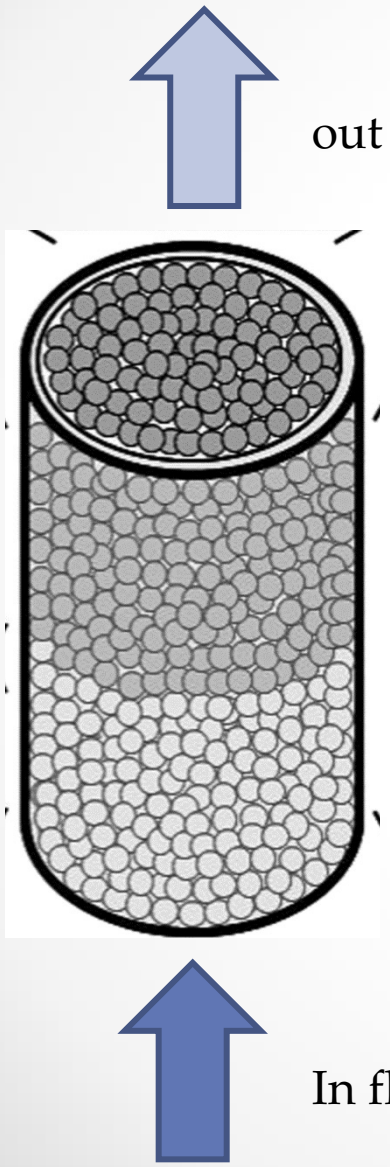
CO_2 chemosorption is widely used in

1. inhalation anesthesia
2. Respiratory care
3. hyperbaric chambers
4. underwater diving gear
5. fire safety apparatuses
6. mine rescue equipment.

Introduction

$$Ca(OH)_2 + CO_2 \rightarrow CaCO_3 \downarrow + H_2O$$

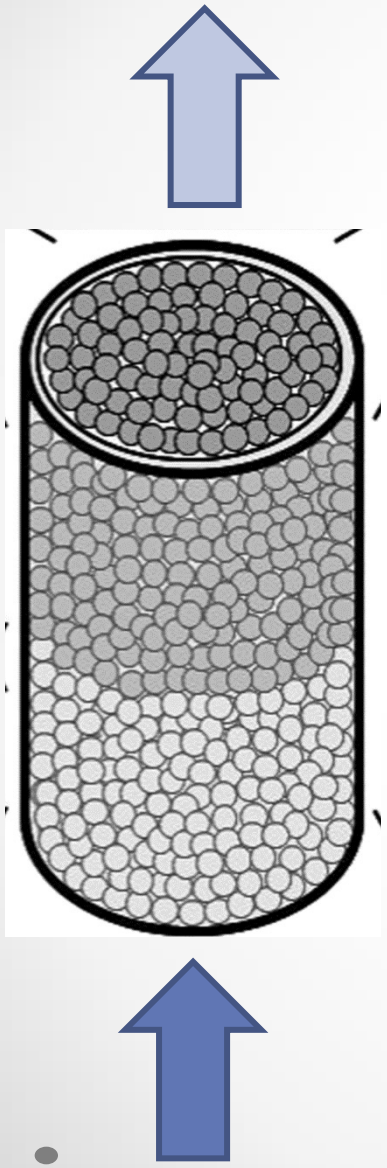
Introduction



Sorption efficiency depends on a number of physical parameters:

1. Pellets packing
2. Pellets shape
3. Internal porosity
4. Pore space structure
5. CO2 concentration at inlet
6. Flow regime
7. ….

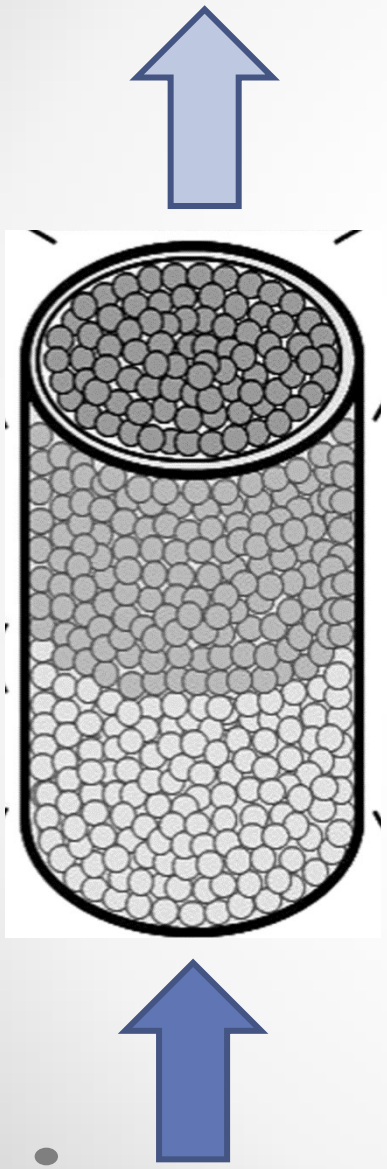
Mathematical model



Assumptions:

1. We deal with double-porosity model with large inter-particle pores and small-scale pores inside the particles
2. Only large-scale pores support the fluid flow
3. The only transport regime in the small-scale pores is the diffusion
4. The considered reaction is the first-order reaction

Mathematical model



Fluid flow

$$\nabla p - \mu \Delta u = 0$$

$$\nabla \cdot u = 0$$

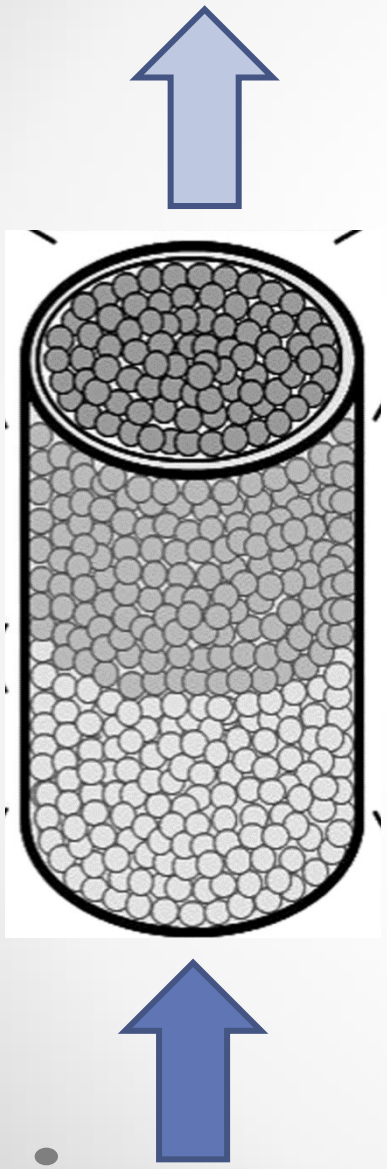
$$x \in \Omega_F$$

Reactive transport

$$\frac{\partial \phi C_j}{\partial t} + \nabla \cdot \left(u C_j \right) - \nabla \cdot \left(D_j \nabla C_j \right) = F_j(C)$$

$$x \in \Omega_F \cup \Omega_G$$

Mathematical model



Reactive transport

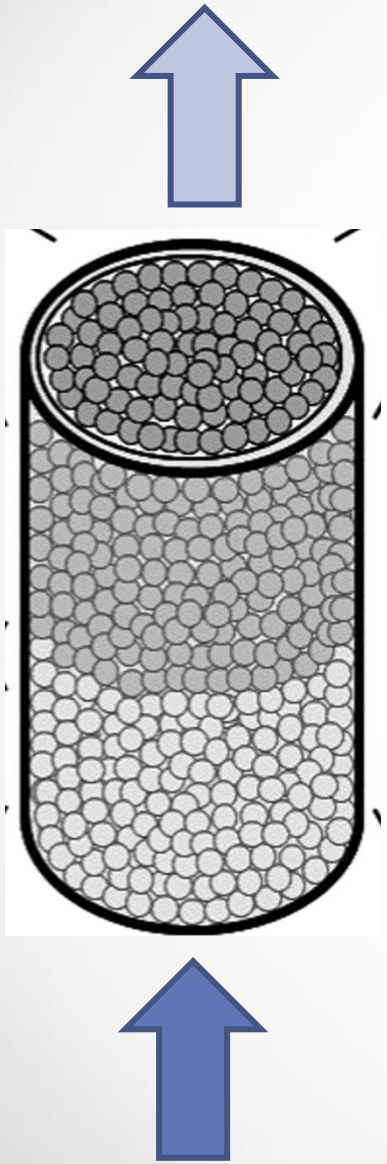
$$\frac{\partial \phi C_{CO_2}}{\partial t} + \nabla \cdot \left(u C_{CO_2} \right) - \nabla \cdot \left(D_{CO_2} \nabla C_{CO_2} \right) = -k \phi C_{CO_2} C_{Ca(OH)_2},$$

$$\frac{\partial \phi C_{H_2O}}{\partial t} + \nabla \cdot \left(u C_{H_2O} \right) - \nabla \cdot \left(D_{H_2O} \nabla C_{H_2O} \right) = k \phi C_{CO_2} C_{Ca(OH)_2},$$

$$\frac{\partial C_{Ca(OH)_2}}{\partial t} = -k \phi C_{CO_2} C_{Ca(OH)_2},$$

$$\frac{\partial C_{CaCO_3}}{\partial t} = k \phi C_{CO_2} C_{Ca(OH)_2},$$

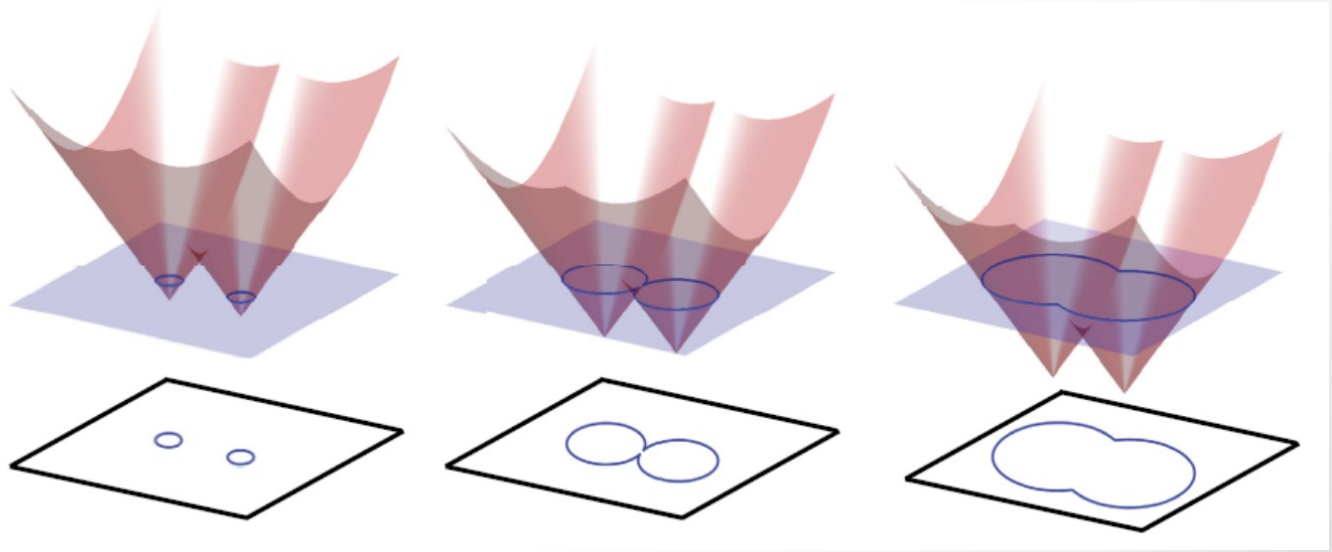
Numerical methods



1. Level-set to represent the model geometry

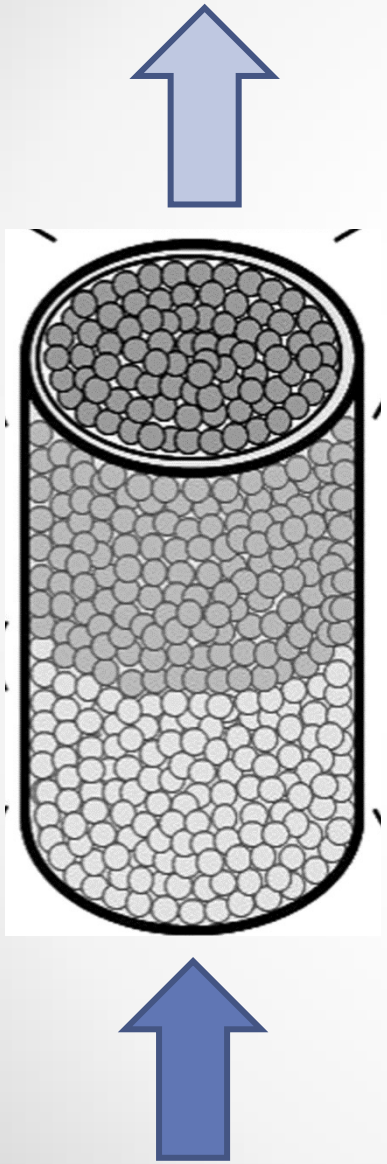
$$\Gamma(\vec{x}) = \left\{ \vec{x} \mid \varphi(\vec{x}, t) = 0 \right\},$$

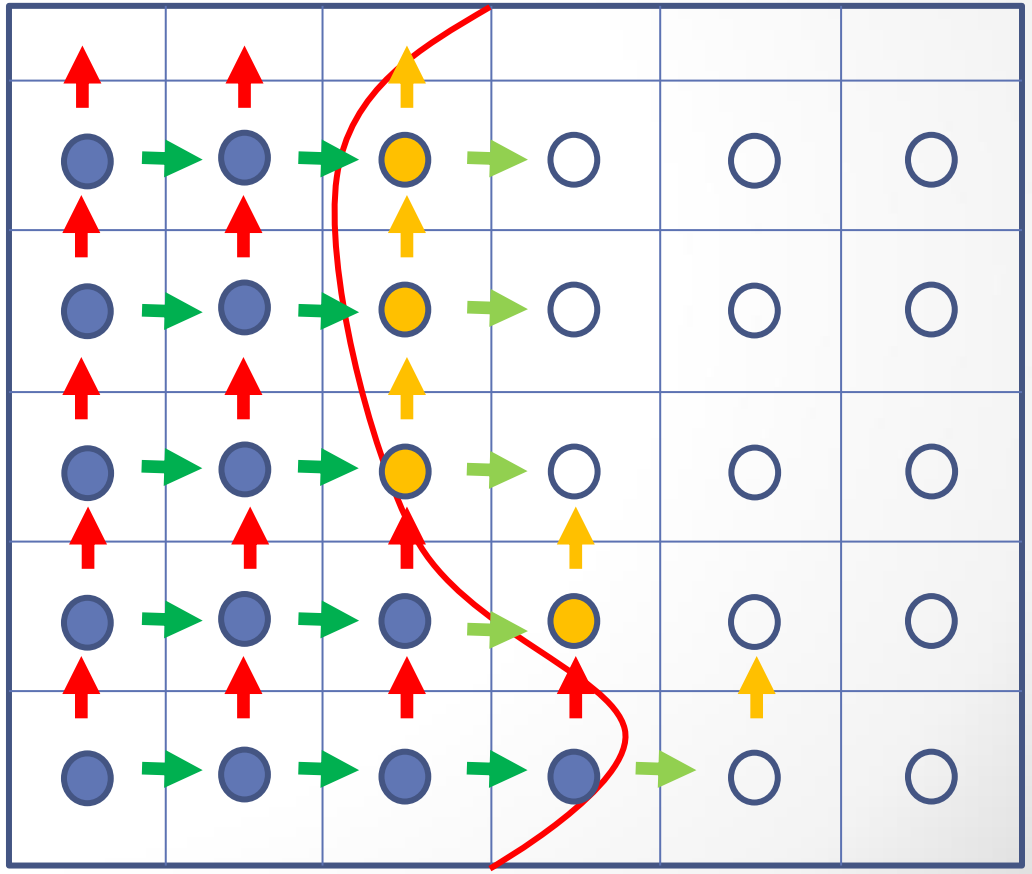
$$\left\| \nabla_x \varphi(\vec{x}, t) \right\| = 1$$



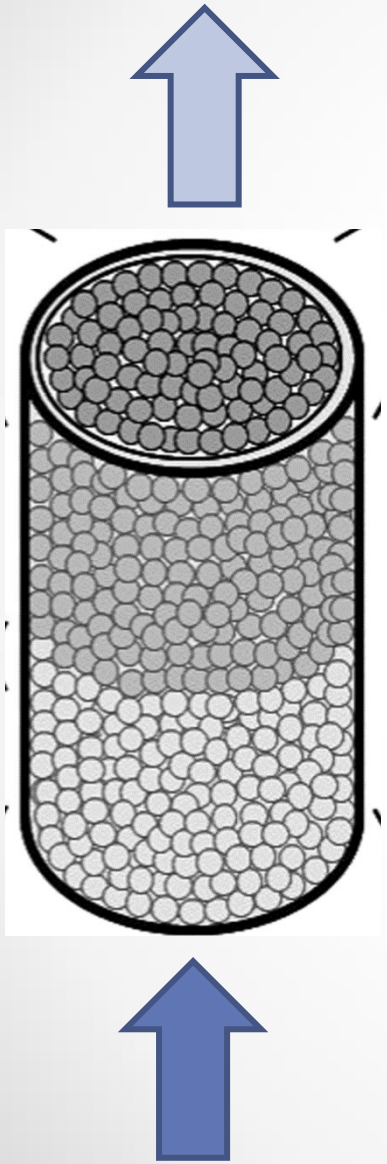
Numerical methods

1. Level-set to represent the model geometry
2. Immersed boundaries to account for irregular geometry





Numerical methods



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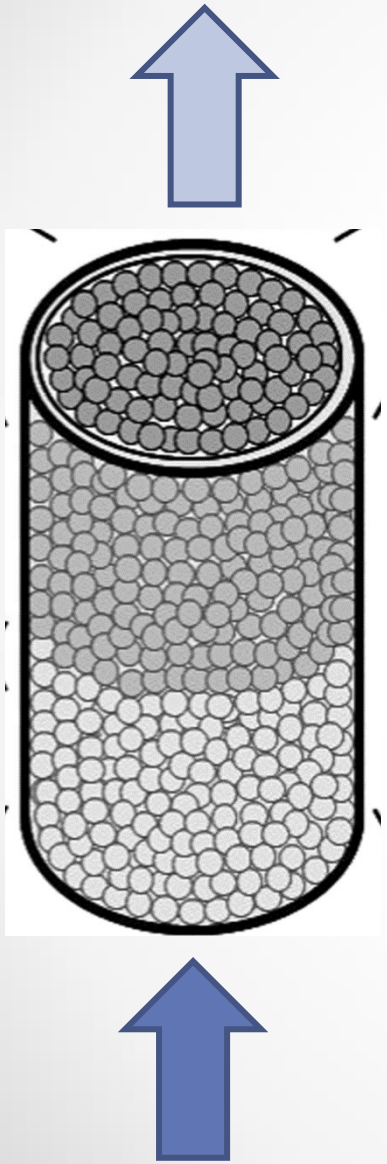
3. Projection-type method to solve Stokes equation with finite-difference approximation

Numerical methods

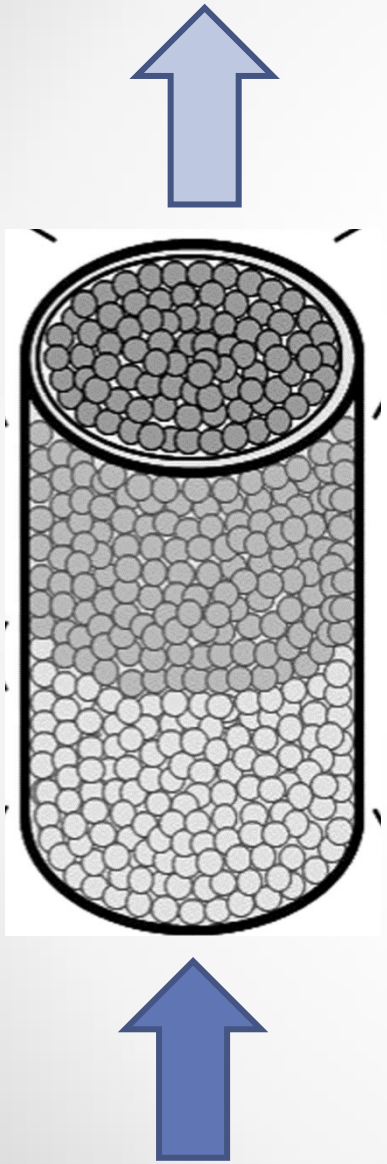


1. Level-set to represent the model geometry
2. Immersed boundaries to account for irregular geometry
3. Projection-type method to solve Stokes equation with finite-difference approximation
4. AD+R splitting scheme to solve advection-diffusion reaction equation.
5. Explicit scheme for AD equation
6. Semi-implicit for R equation

$$\phi \frac{C_j^{n+1/2} - C_j^n}{\tau} + \nabla_h \cdot \left(u C_j^n \right) - \nabla_h \cdot \left(D_j \nabla_h C_j^n \right) = 0$$

$$\frac{C_j^{n+1} - C_j^{n+1/2}}{\tau} = F_j(C^{n+1}, C^{n+1/2})$$

Numerical methods



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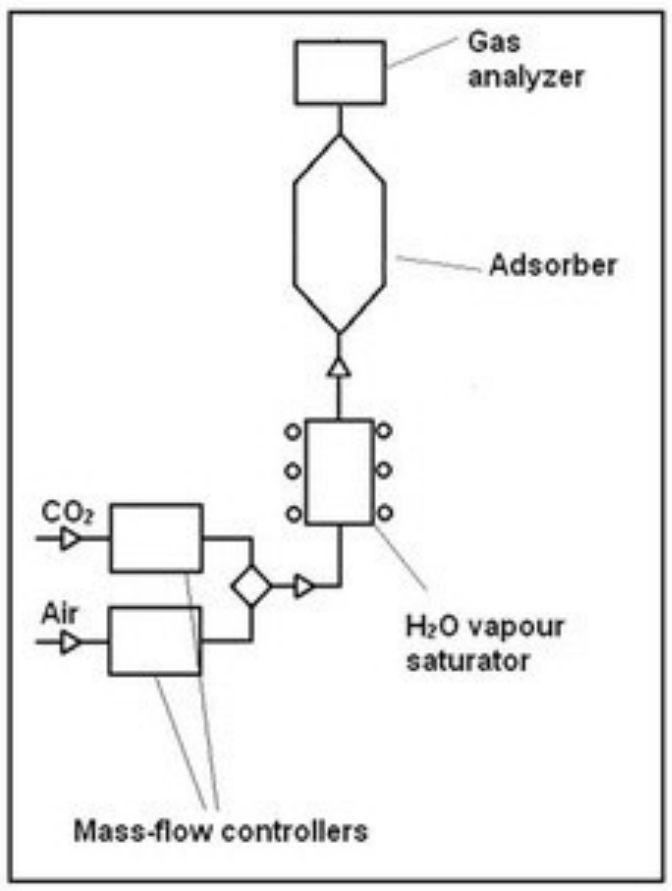
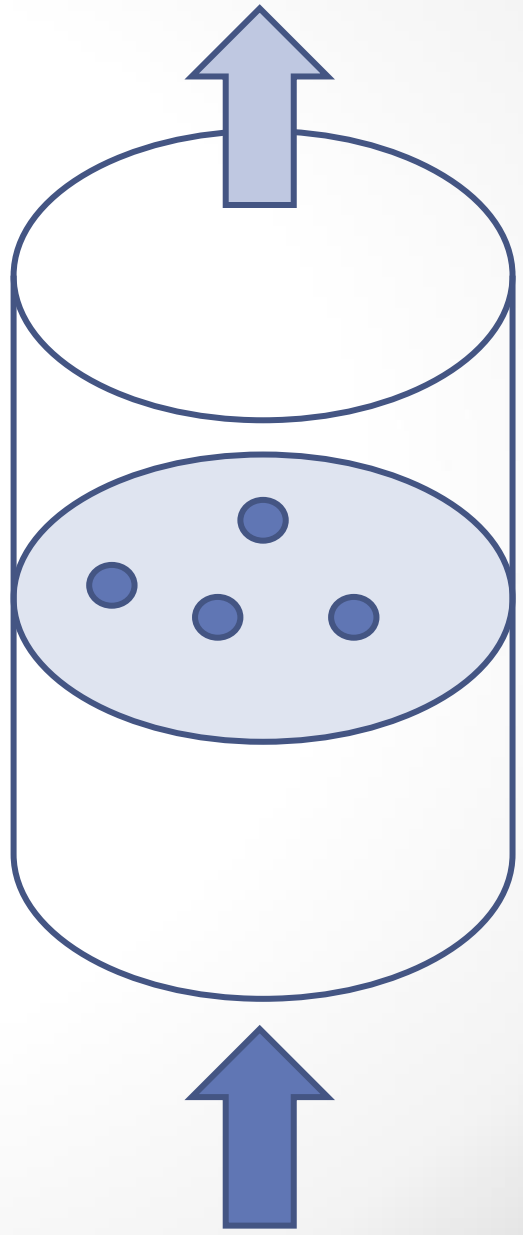
$$\frac{C_{CO_2}^{n+1} - C_{CO_2}^{n+1/2}}{\tau} = -kC_{CO_2}^{n+1} C_{Ca(OH)_2}^{n+1/2},$$

$$\frac{C_{Ca(OH)_2}^{n+1} - C_{Ca(OH)_2}^{n+1/2}}{\tau} = -\phi kC_{CO_2}^{n+1/2} C_{Ca(OH)_2}^{n+1},$$

$$\frac{C_{CaCO_3}^{n+1} - C_{CaCO_3}^{n+1/2}}{\tau} = -\phi kC_{CO_2}^{n+1} C_{Ca(OH)_2}^{n+1}.$$

Experiments





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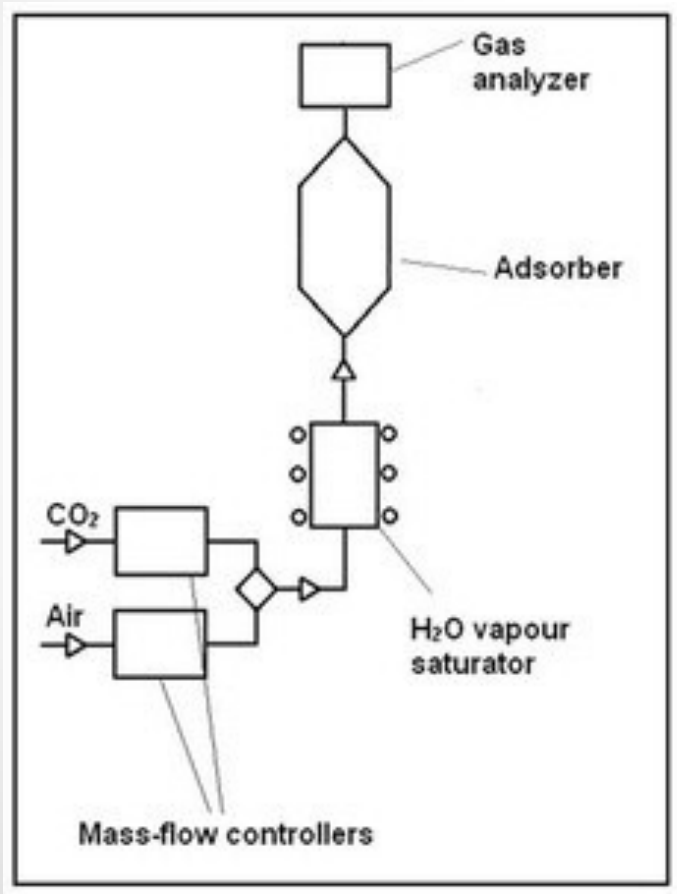


CO_2 concentration 5%				
	$t = 0$	$t = 15$	$t = 30$	$t = 60$
$\mu_{Ca(OH)_2}$	0.76	0.32	0.19	0.13
μ_{CaCO_3}	0.05	0.5	0.72	0.78

CO_2 concentration 1%				
	$t = 0$	$t = 15$	$t = 30$	$t = 60$
$\mu_{Ca(OH)_2}$	0.6948	0.4604	0.3535	0.2672
μ_{CaCO_3}	0.0522	0.2318	0.3818	0.475

Numerical experiments

$$\frac{\partial \phi C_{CO_2}}{\partial t} + \nabla \cdot \left(u C_{CO_2} \right) - \nabla \cdot \left(D_{CO_2} \nabla C_{CO_2} \right) = -k \phi C_{CO_2} C_{Ca(OH)_2},$$

$$\frac{\partial C_{Ca(OH)_2}}{\partial t} = -k \phi C_{CO_2} C_{Ca(OH)_2},$$

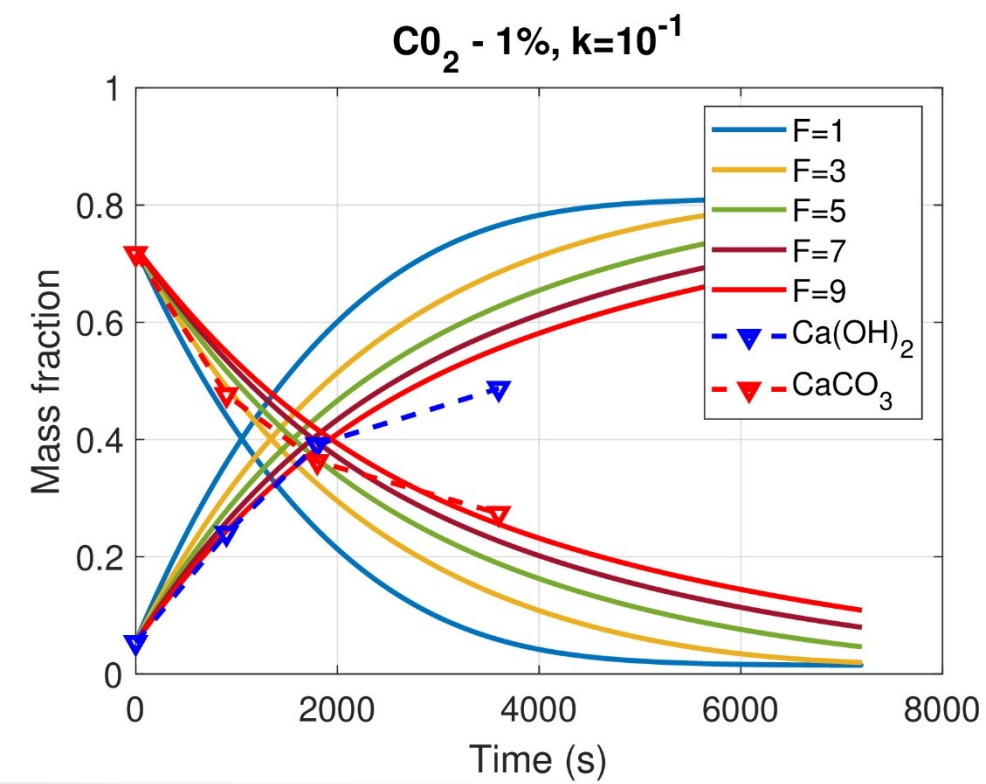
$$\frac{\partial C_{CaCO_3}}{\partial t} = k \phi C_{CO_2} C_{Ca(OH)_2}.$$

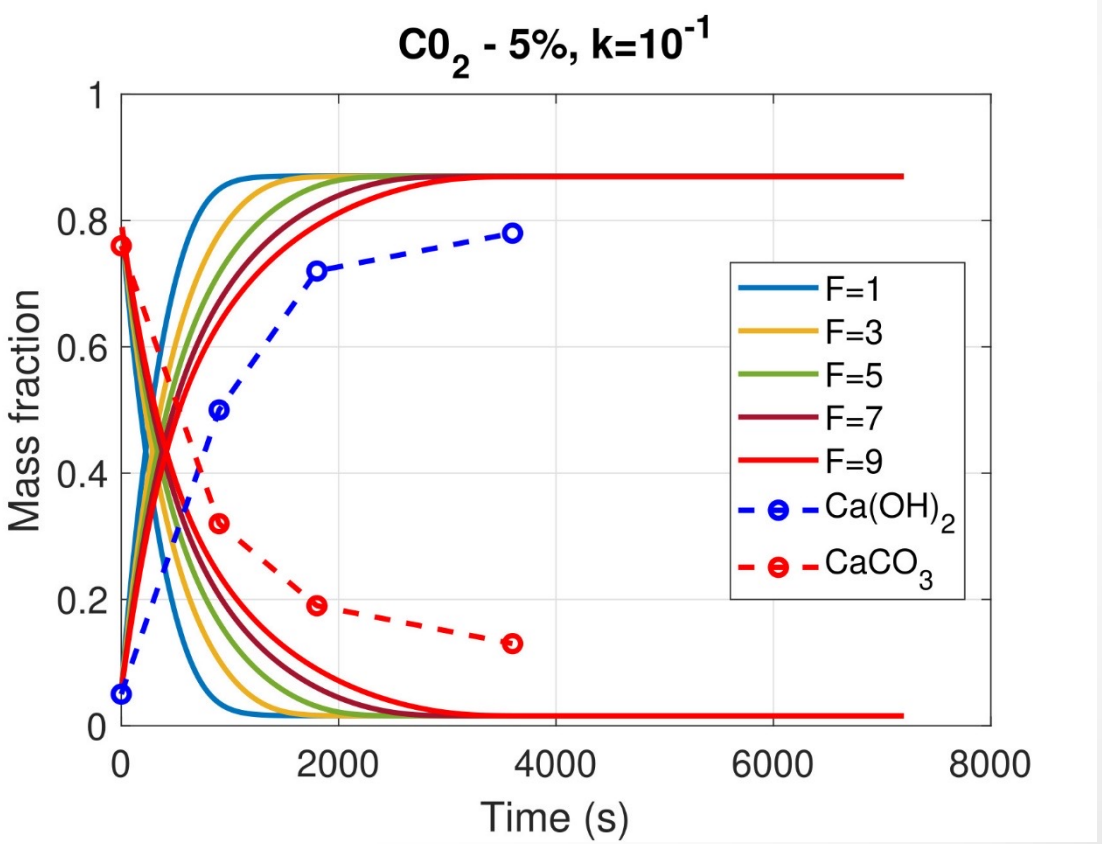
We do not know two parameters:

1. Reaction rate
2. Formation factor of the microporous space

$$D_{CO_2} = \frac{D^0_{CO_2}}{F}$$

Numerical experiments





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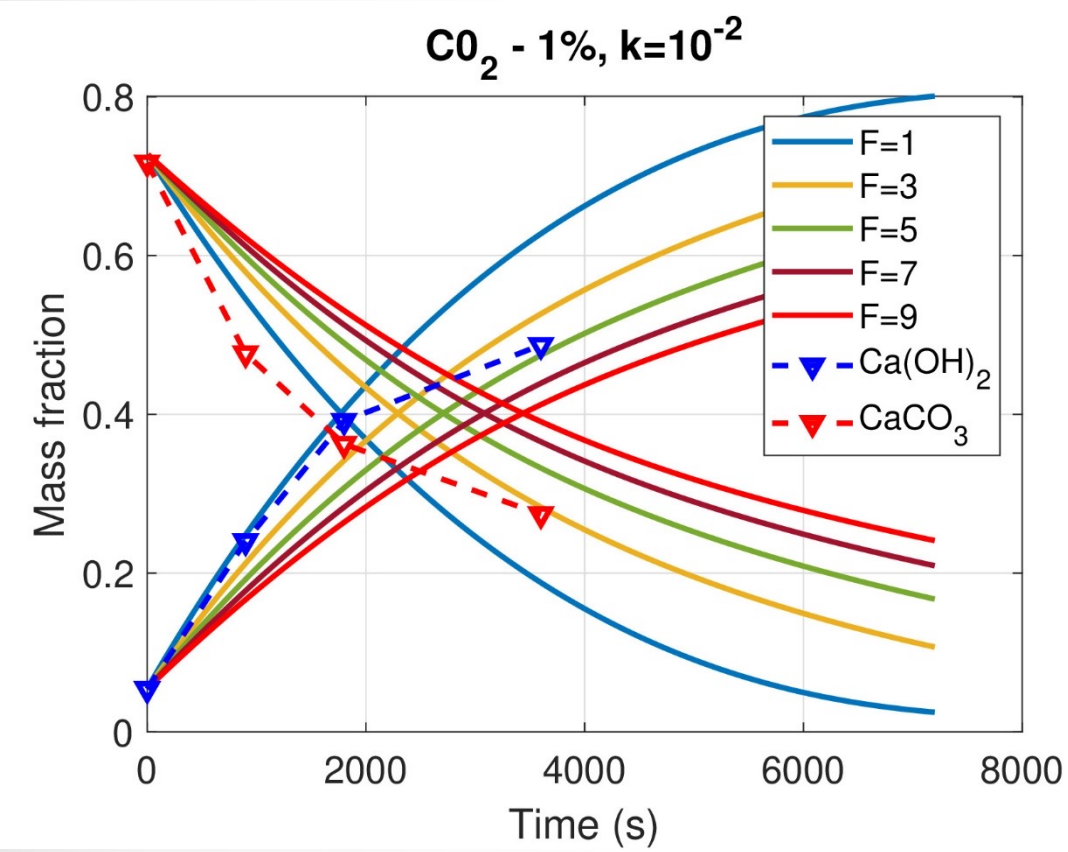
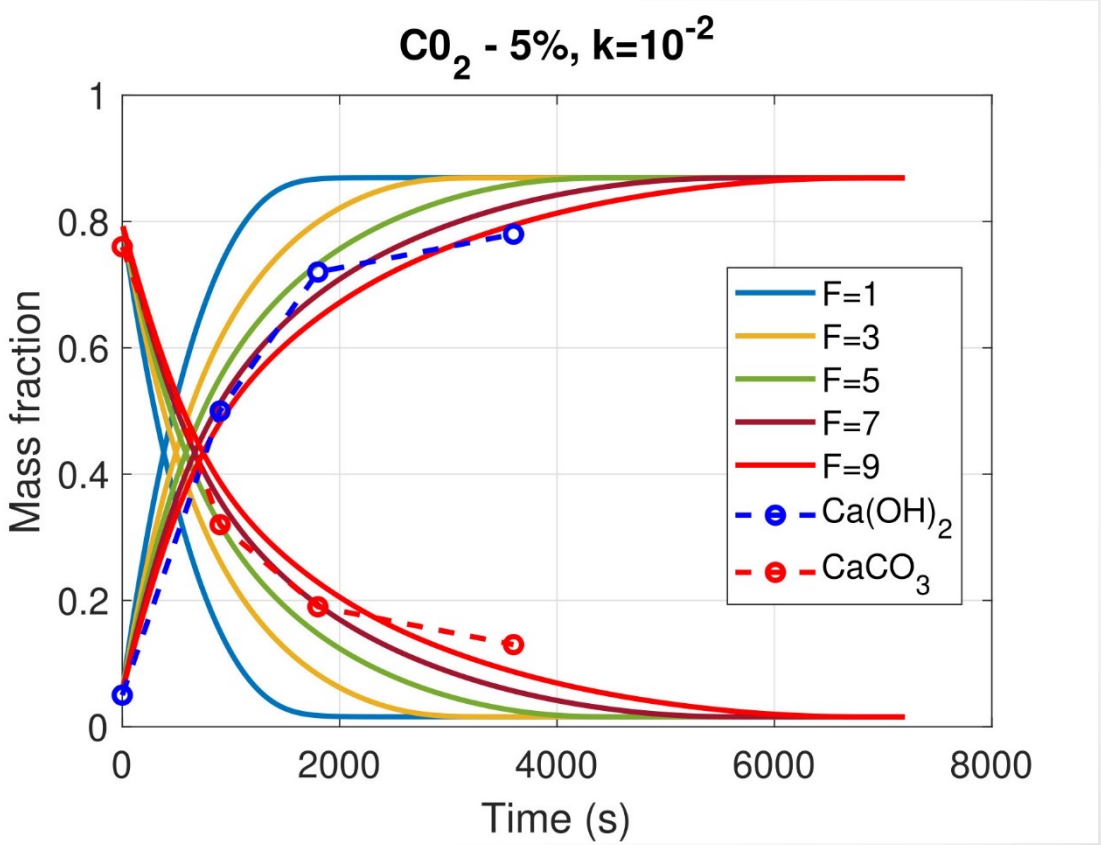
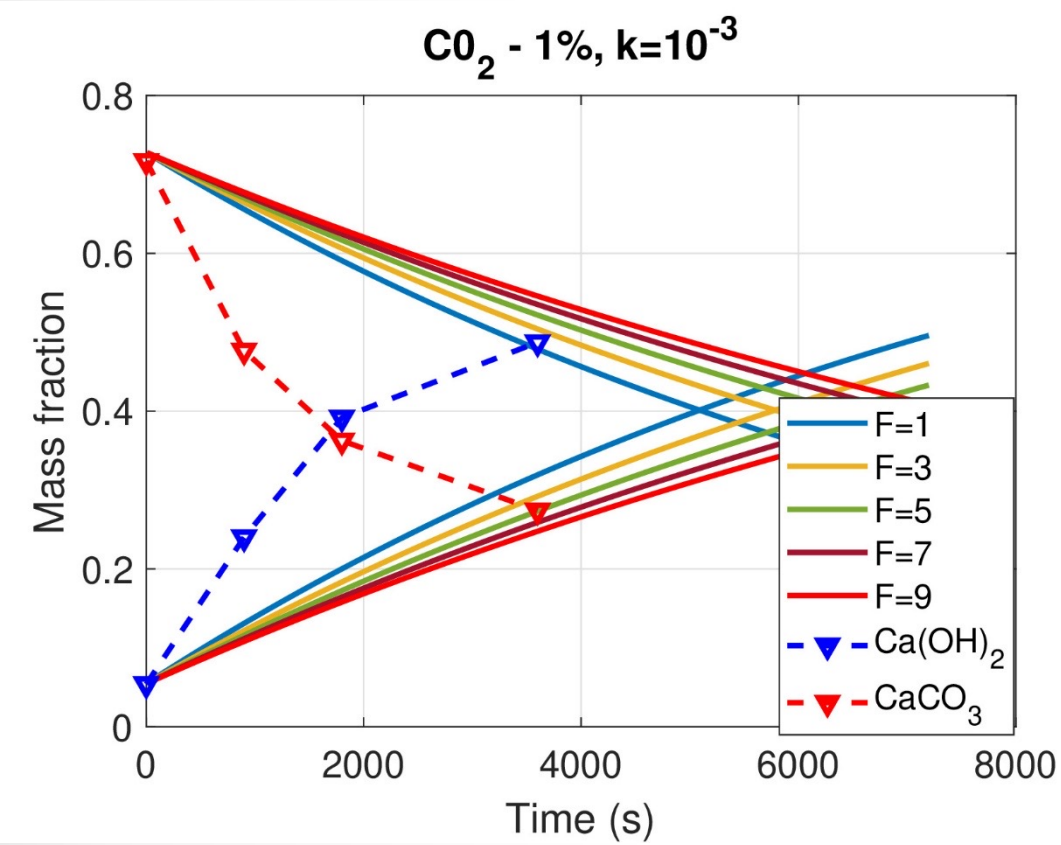
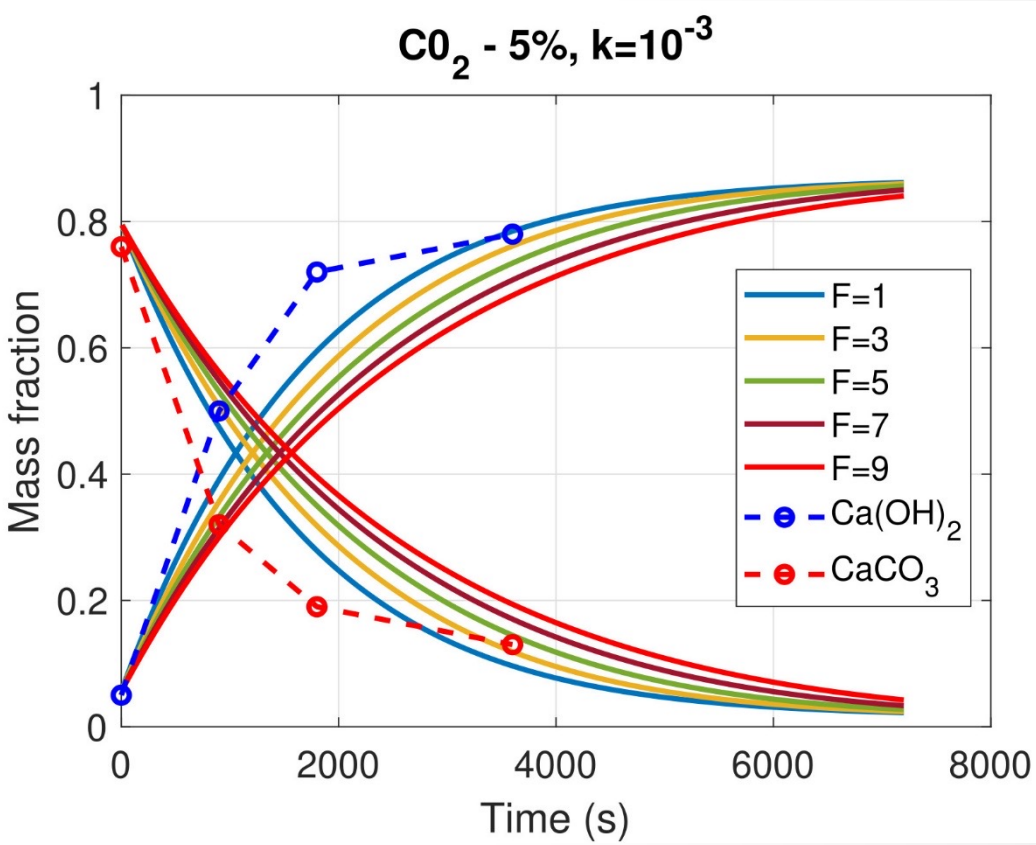




Numerical experiments





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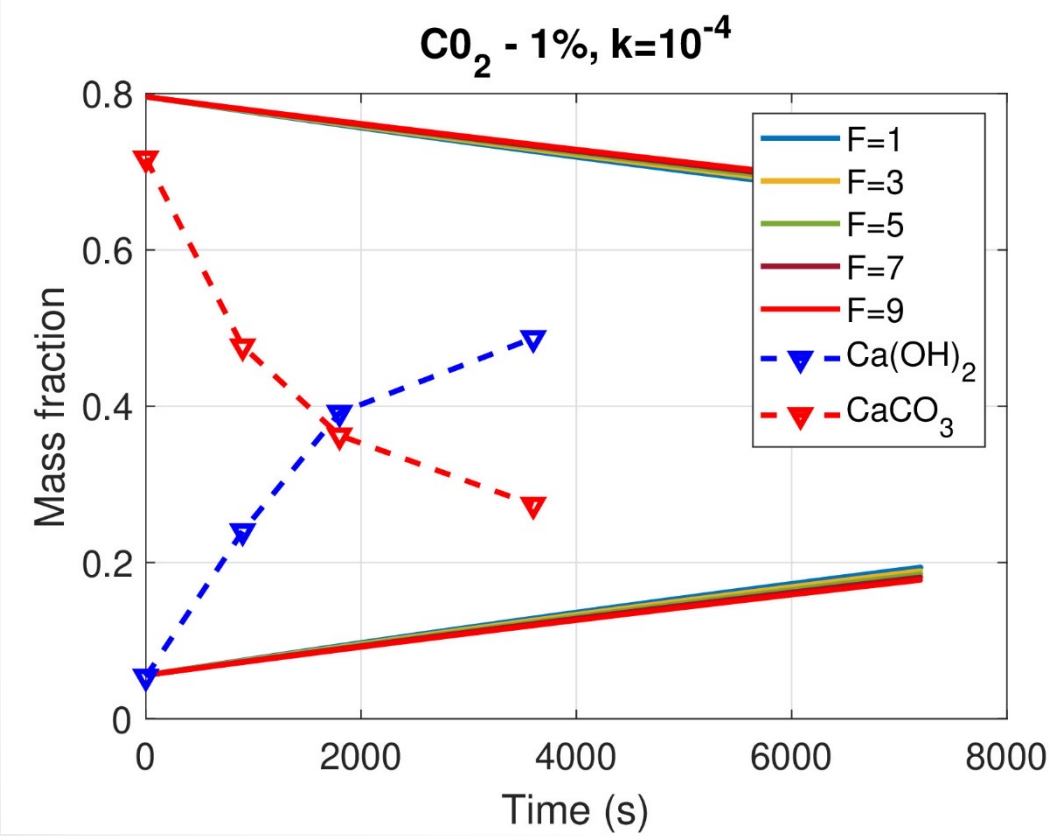
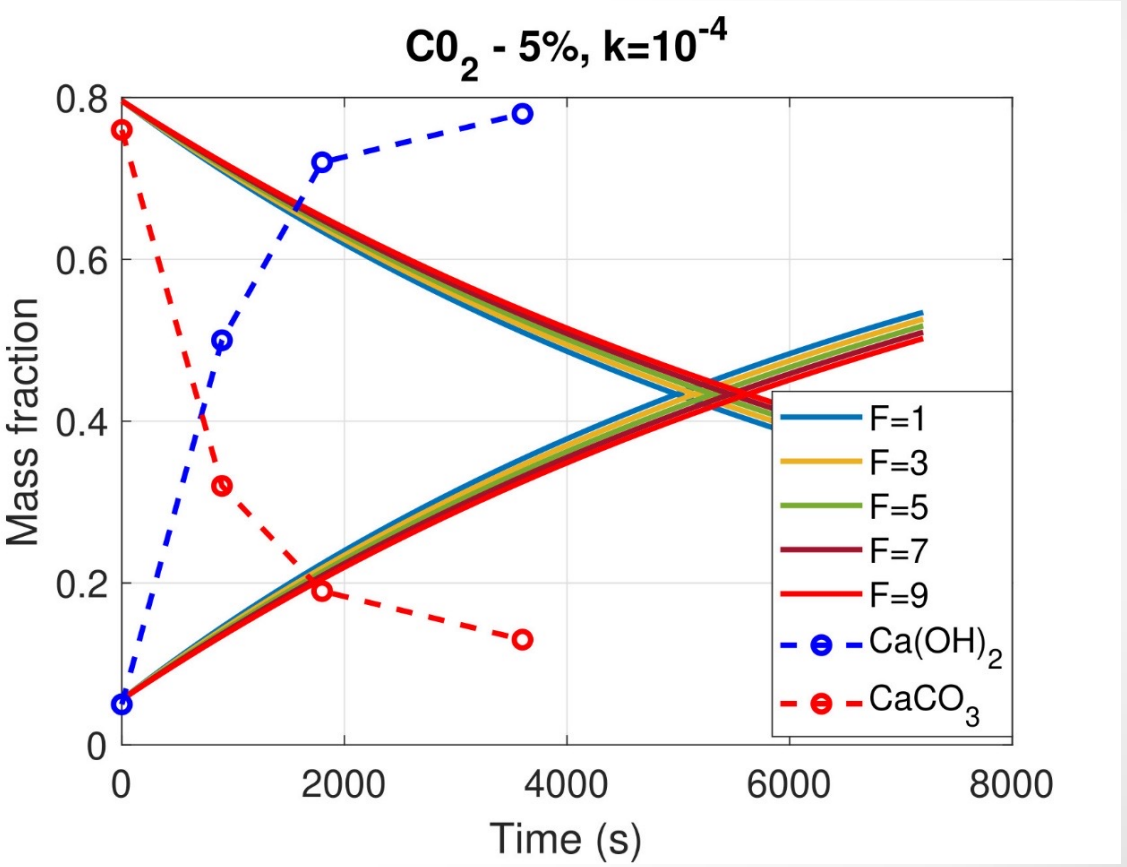
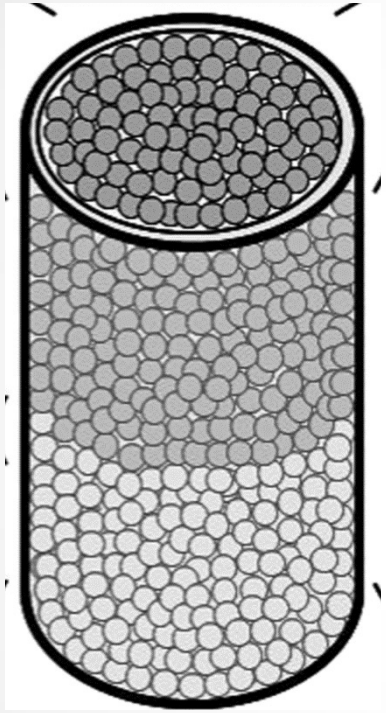




CO2 break-through

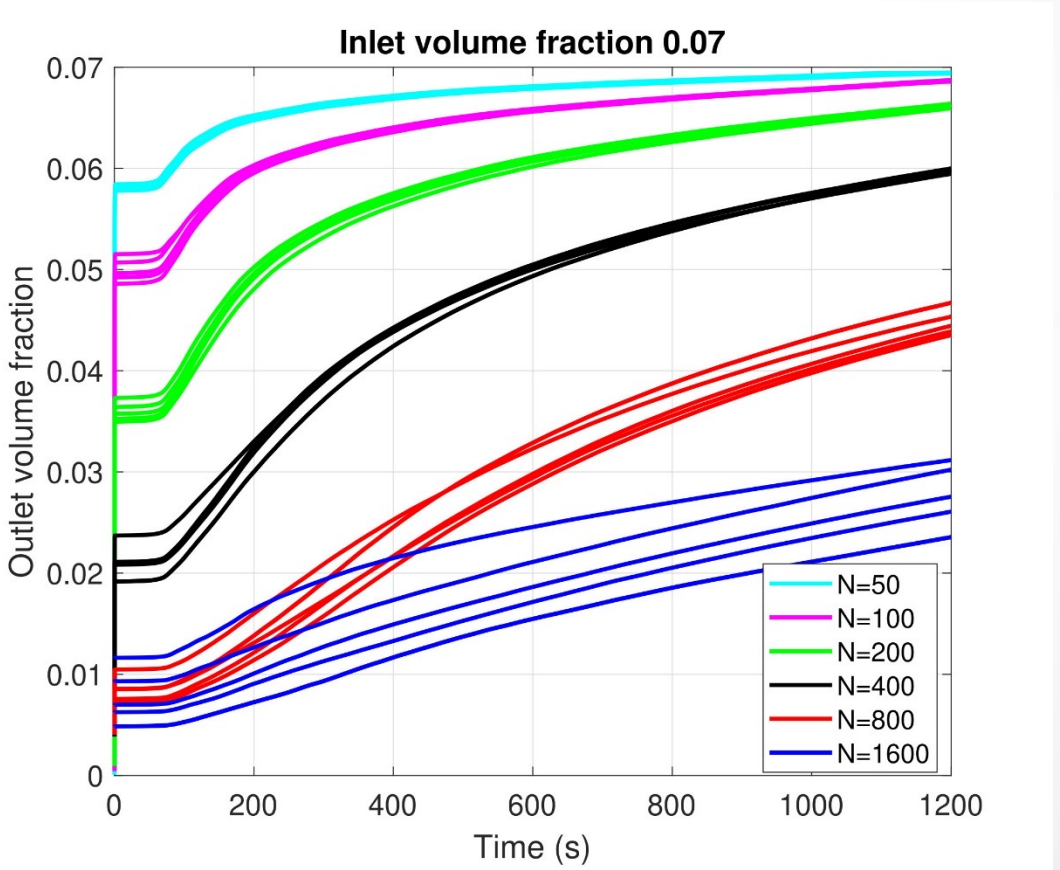
30 cm



30 cm

$7.5 \cdot 10^{-5} m^3 / s$

Particle size 3 mm
Number of particles 50, 100, 200, 400, 800, 1600
Grid step 0.3 mm



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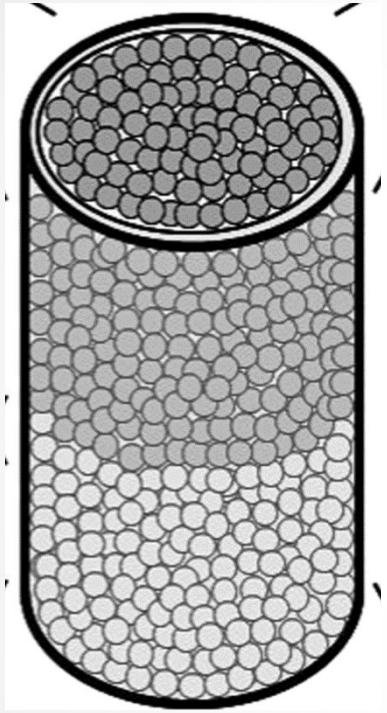

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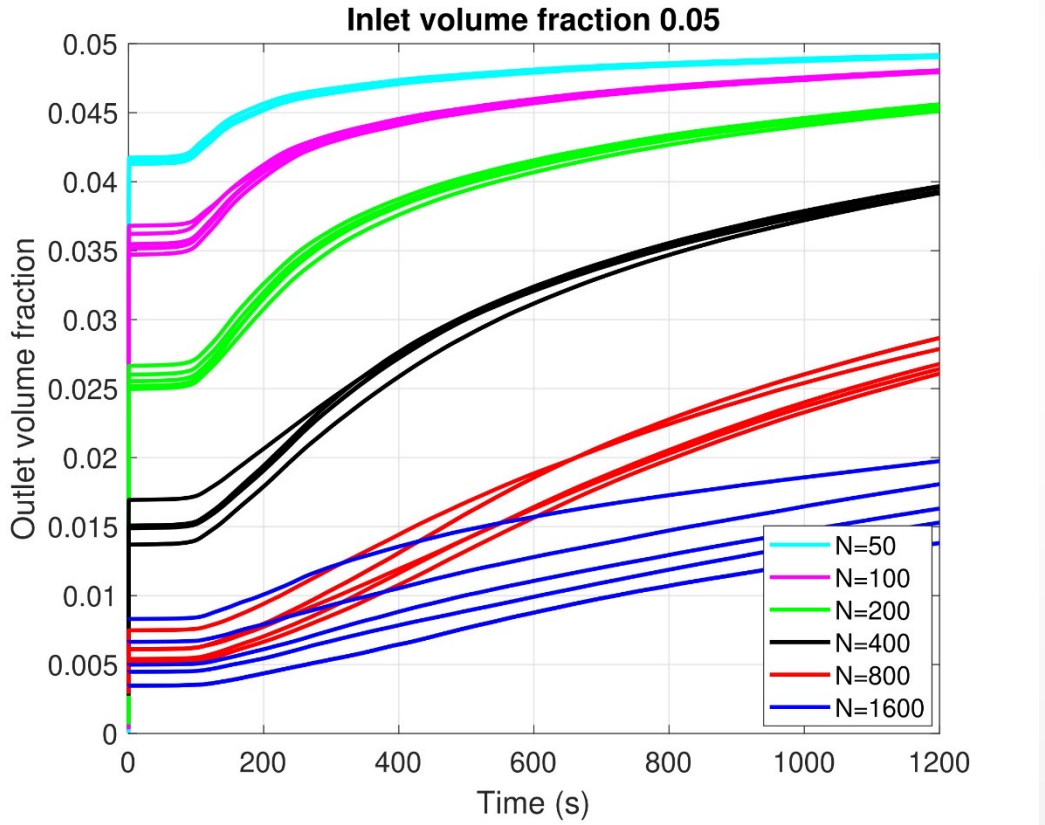

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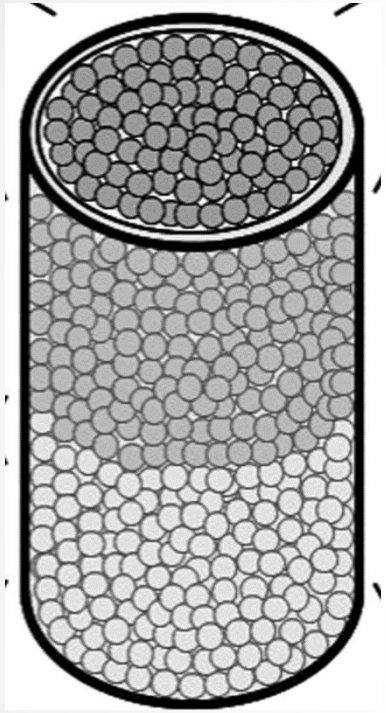

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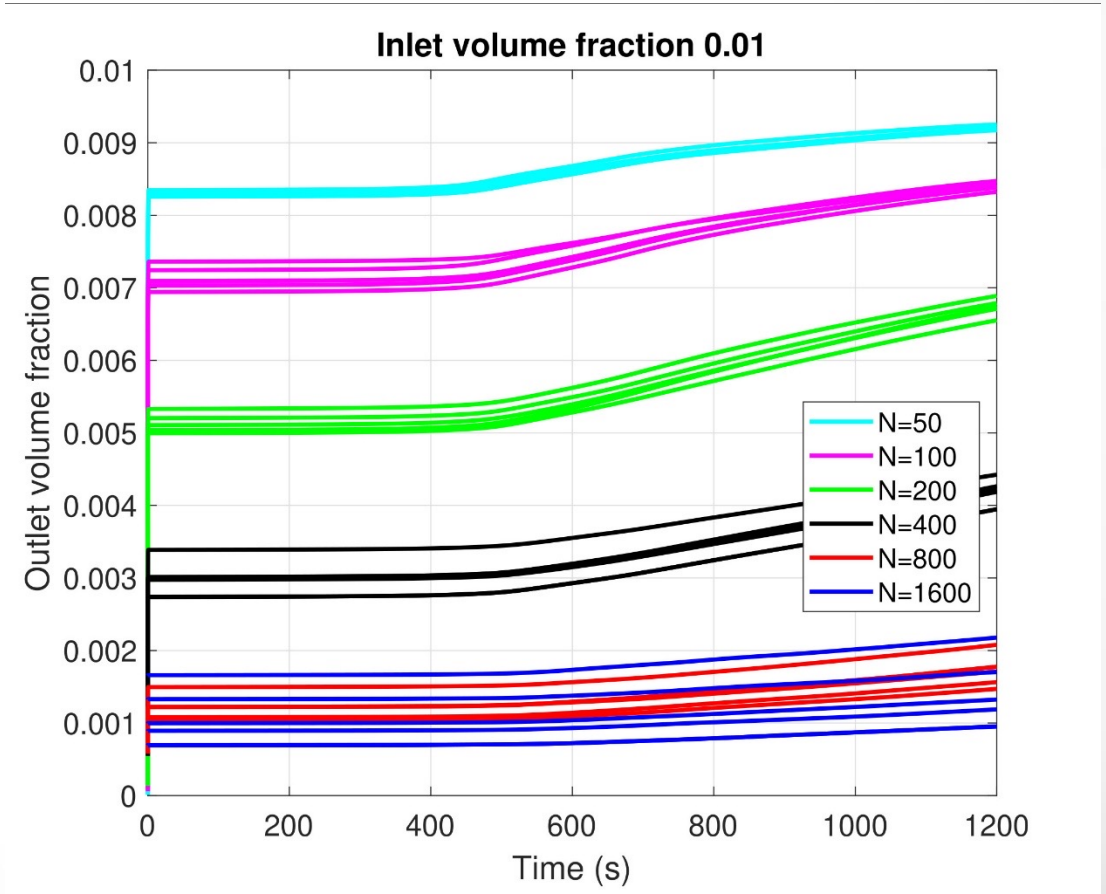

Conclusions

1. We presented an algorithm for numerical simulation of CO2 chemosorption.

2. The algorithm is implemented using CUDA technology and allows simulating real-size gas reactors using a single GPU.

3. We calibrate the unknown model parameters – reaction rate and the microporous space tortuosity to match the lab experiments.

4. We illustrate that the high density of sorbent particles packing increases the break-though time until the CO2 diffusion rate starts limiting the reaction.

Thank you for attention!