Multiscale Simulation for Net-Zero Carbon Capture in MOF-Based Porous Media

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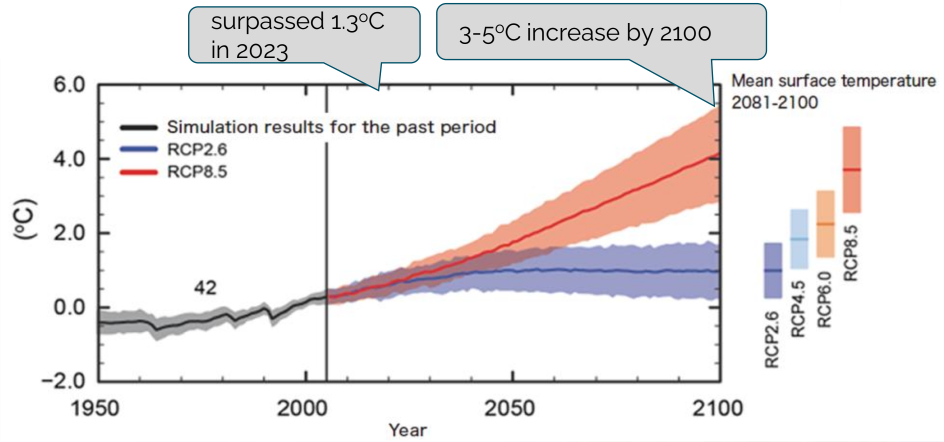
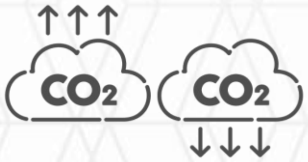
Global Decarbonization Trends: Low-Carbon Energy Solutions

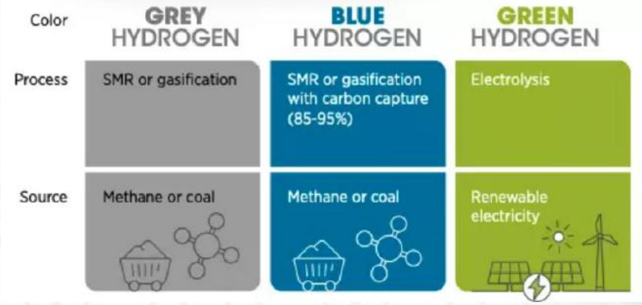
- CO_2 emissions are the primary driver of global climate change
- **Paris agreement**: CO_2 emission reduction
  - Keep temperature rise below 2°C, preferably 1.5°C
  - Already above 1.2°C, on track to pass 1.5°C by 2030
- The **energy sector** is a source of around **75% of GHG** today
- <u>Need for a **cleaner energy** system</u>



Global surface temperature continue to increase

- 50% of CO_2 reduction from **four technology value chains**:
  - ✓ Electrification
  - ✓ Hydrogen
  - ✓ **CCUS**
  - ✓ Bioenergy





Color	GREY HYDROGEN	BLUE HYDROGEN	GREEN HYDROGEN
Process	SMR or gasification	SMR or gasification with carbon capture (85-95%)	Electrolysis
Source	Methane or coal	Methane or coal	Renewable electricity

Simulation is playing a vital role in helping industries transformation to green energy effectively

CADIT Global

Company Profile 2026

Found since 1991

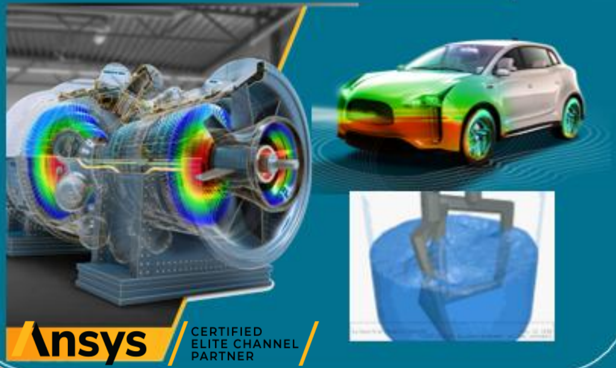
Vision

To Lead the global shift to Industry 4.0 by delivering digital transformation solutions that create exceptional value for our customers, keeping industry best practices in mind & a God centered culture at heart.

Mission

To Empower companies to achieve greater innovation and efficiency through digital transformation solutions & helping clients across the globe reduce costs and time-to-market as your key global partner.

Engineering Simulation

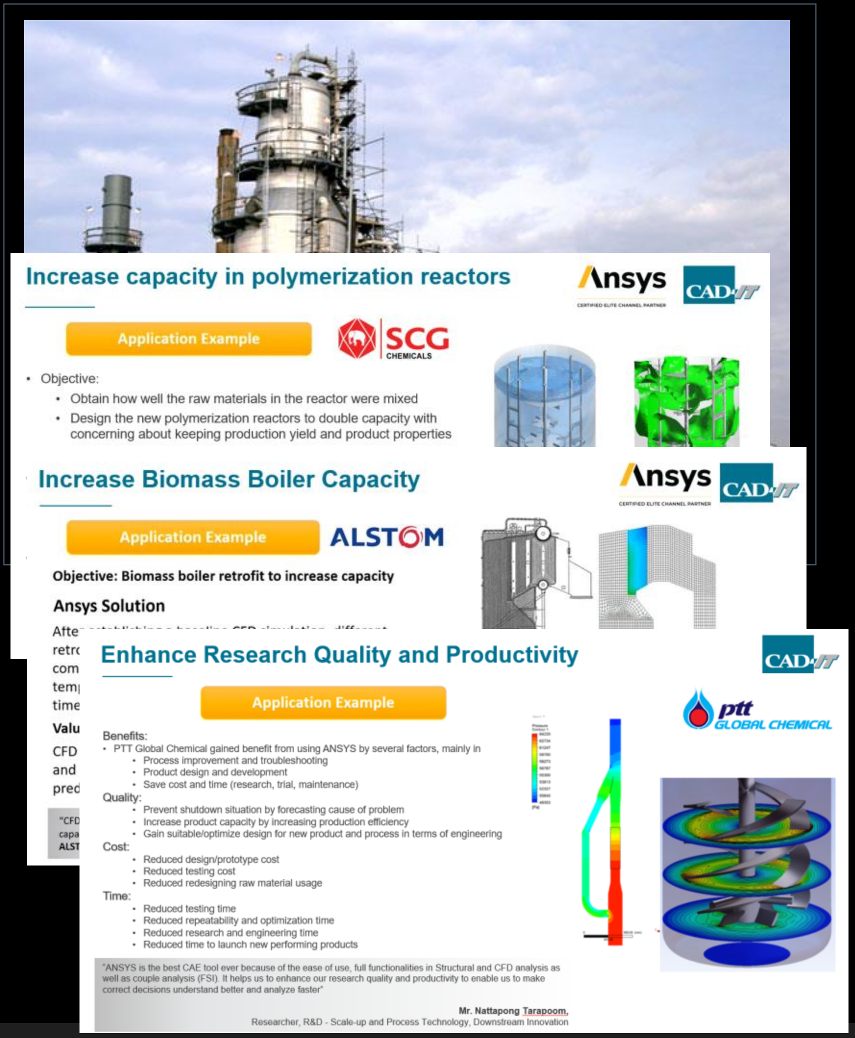


Industry 4.0

Digital Twin

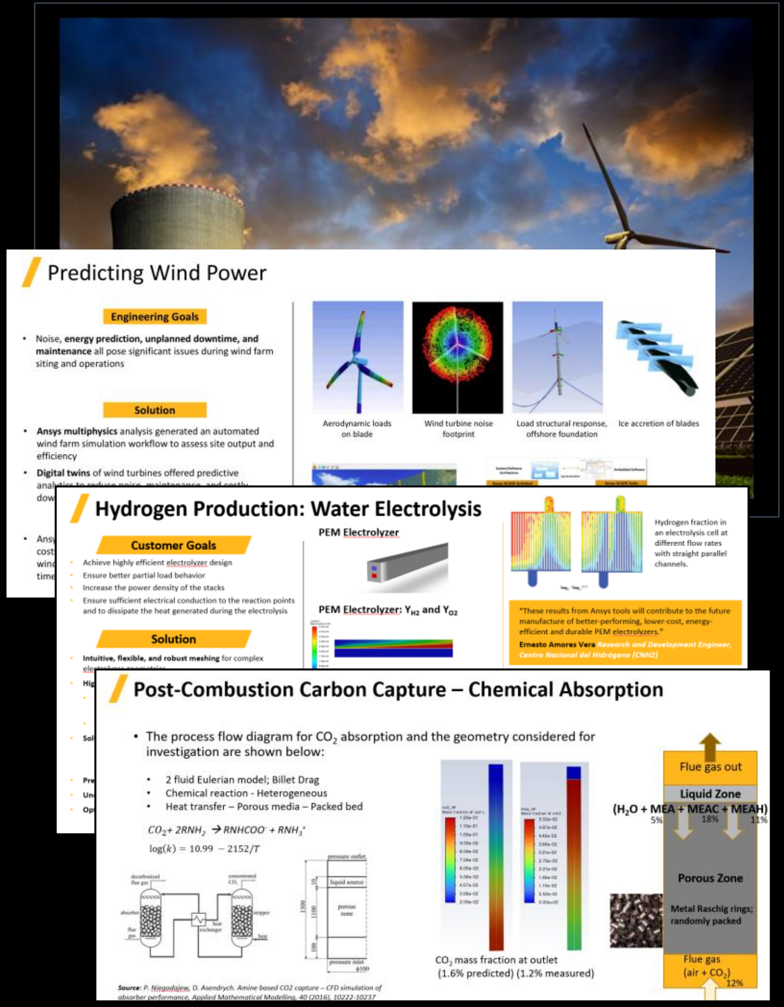
Ansys Energy & Industrials Focused Pillars and Case Studies

1 Efficiency Improvements



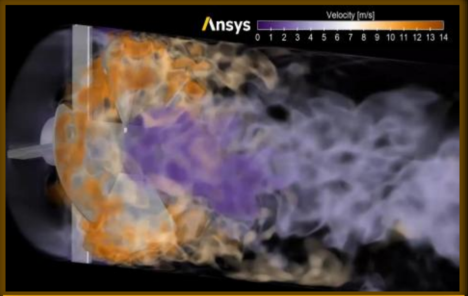
2 Improving Reliability & Affordability

3 Maturing Low Carbon Solutions



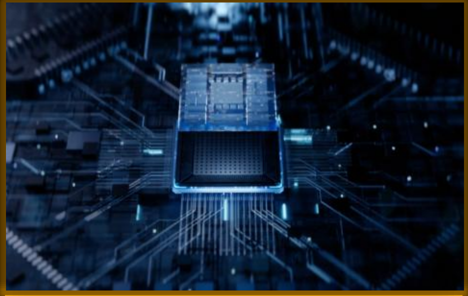
4 Digital Engineering | "Tailwind" Technologies & Ansys Investments

Core Physics Numerical Methods and Models



- Solver methods
- Geometry and meshing
- Shape and topology optimization
- Advanced analysis
- Multi-physics
- Multi-scale

High-Performance Computing

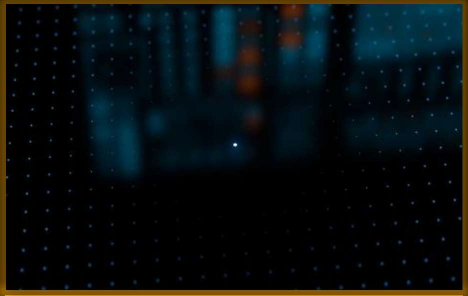


- Shared-memory
- Message-passing
- Fine-grained GPUs
- New architectures: FPGAs & AI hardware
- Quantum computing

Artificial Intelligence and Machine Learning

- Solver acceleration
- Solver settings
- Top-down methods
- Bottom-up methods
- Reduced order models
- Generative AI

Cloud, Platform, and User Experience



- Cloud Enabled
- Cloud Native
- Platform, Collaboration
- Open APIs and developer ecosystem
- Common user experience

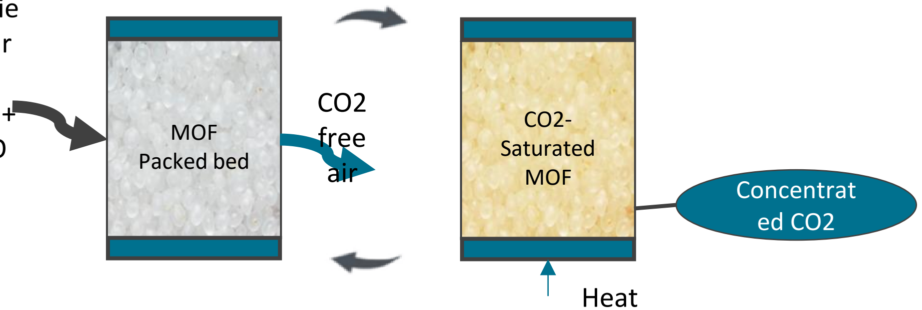
Digital Engineering

- Model Based System Eng.
- Requirements & architecture Connections
- Safety, security, & software
- Digital twins
- Simulation process & data management
- Mission engineering

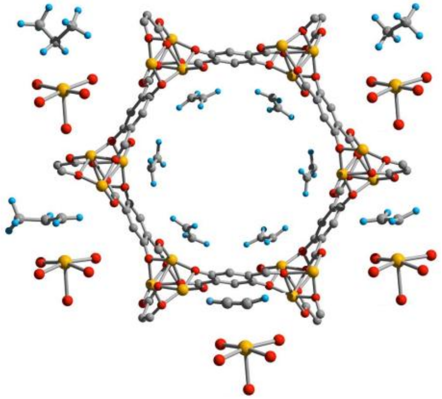
The Digital Transformation Will Accelerate Pillars #1, #2 & #3 and Drive Scaling ...

Background: Carbon Capture in Particle-Bed Reactors

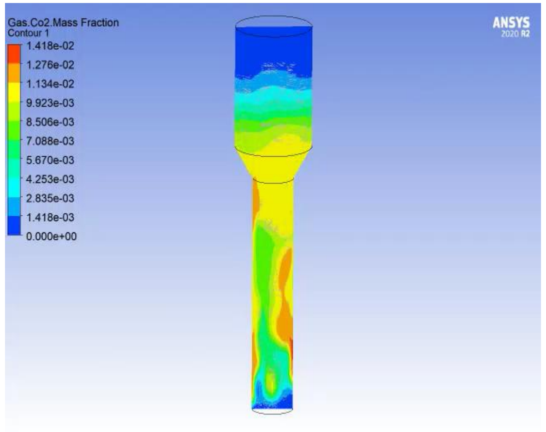
- Particle-bed reactors are widely used in chemical process industries, such as for the process of capturing carbon dioxide.
- Carbon capture using **particle-bed reactors** involves passing **CO_2-containing gas (flue gas)** through a bed of **solid particles (sorbents). MOF materials** are commonly used for these applications;
- Metal-Organic Frameworks (MOFs) are coordination polymers with properties such as permanent microporosity that enable applications such as **gas adsorption**;
- Adsorption is a surface process that leads to transfer of a molecule from a fluid bulk to solid surface, due to physical forces or chemical bonds. It is usually reversible (desorption).
- **The capture of the physics in such processes require coupled DEM-CFD simulations to analyze species adsorption and desorption throughout the MOF along the particle bed reactors.**



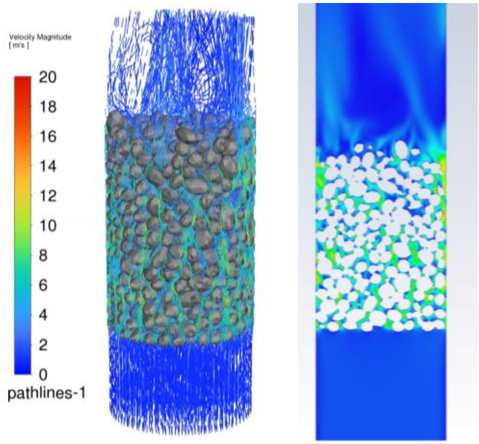
Simplified Adsorption/Desorption processes



Metal-organic-framework materials act as a sponge to capture the CO2 chemically



Solution for CO_2 distribution in dense fluidized bed for FCC regenerator

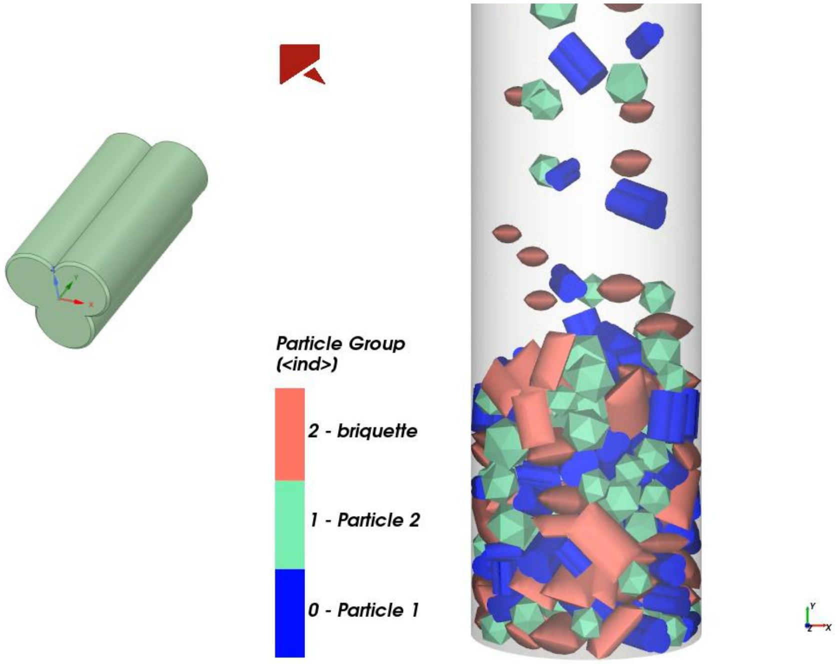


Fixed Bed Reactor

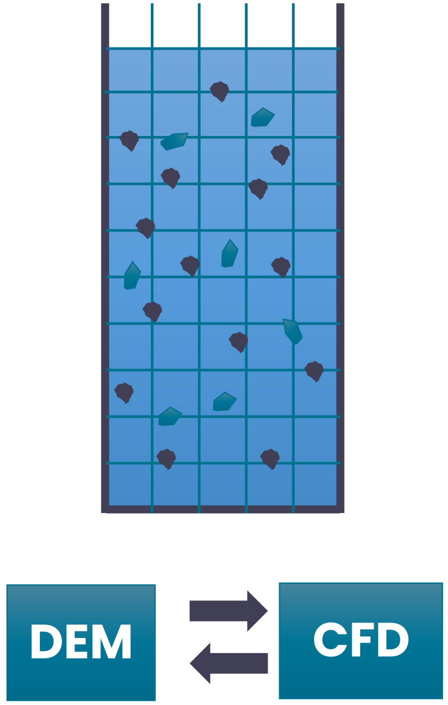
Multiscale Simulation of Gas-Solid Flows:
CFD-DEM Coupling

/ Ansys Rocky (DEM)

Rocky enables the creation of porous media made of particle beds

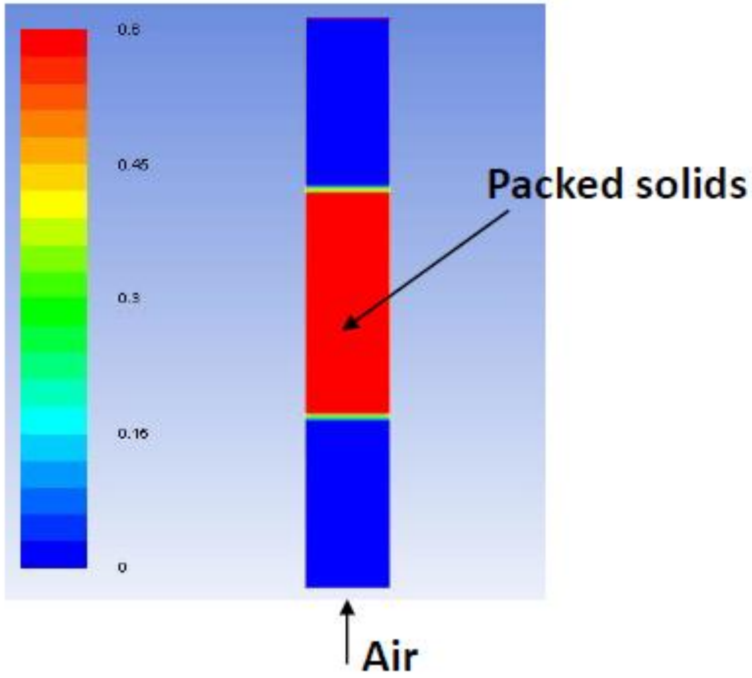


MICROSCALE (Particle-resolved): Volume Fraction, Momentum and Heat exchange terms



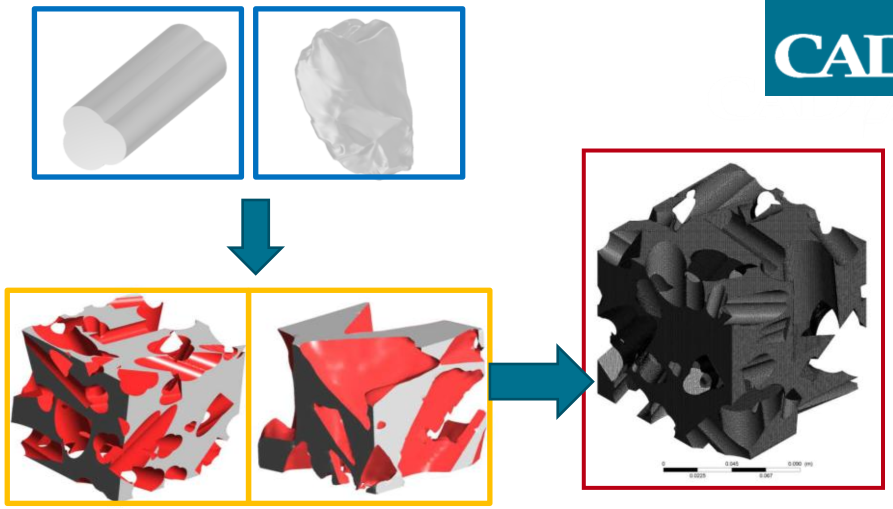
/ Ansys Fluent (CFD)

Fluent allows for predicting the pressure drop over different porous domains exported from Rocky



MACROSCALE (Fluid-resolved): Two-fluid averaged equation approach : Fluid Velocity and Pressure Fields

Complexity & Simulation Challenges



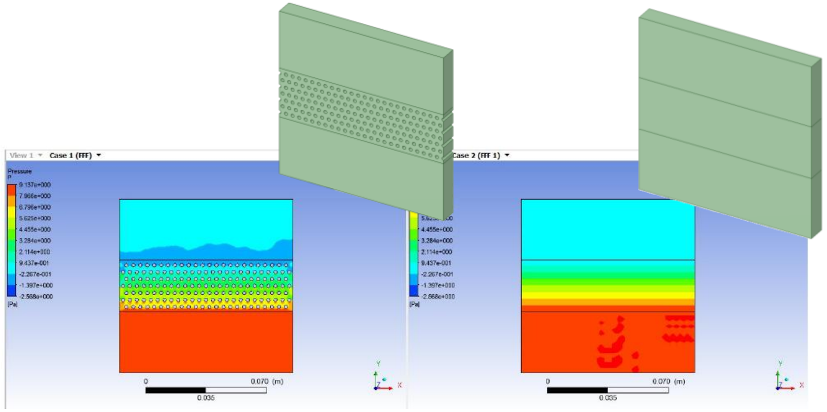
Engineering Goals

- Evaluate the performance of Metal-Organic Frameworks (MOFs) on adsorption of carbon dioxide from ambient air and desorption processes.
- Predict particle bed porosity and permeability.
- Evaluate effects of particle swelling/deswelling on pressure drop and porosity.

Complexity & Simulation Challenges

Devices are very complex

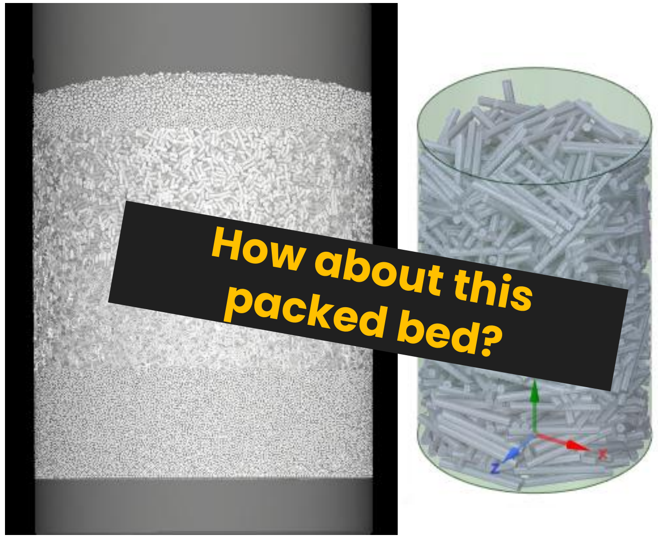
- Scale bridging (particle → reactor)
- Complex geometry: how to represent the porosity and permeability properties of particle beds
- Complex mesh
- Complex boundary conditions
- Complex physics: Turbulence; Multiphase flow (gas–solid interaction); Chemistry



Uniform Bed

Porous Media Approach to model the flow across the bed using Darcy–Forchheimer law

- Reducing a lot the computational cost
- Include heat and mass transfer



Ansys Solution with CFD-DEM Coupling

Particle bed generation in Rocky

- Particle bed generation with real particle shape of the MOF
- Particle bed exported as .stl (geometry) and .csv (position/orientation final state) files

Reference data creation & validation

- Mesh created using the particle bed geometry
- ΔP vs. Fluid inlet velocity curve created to generate reference standalone CFD data
- DEM-CFD Coupled simulation run to calibrate drag laws

Solver customization

- Ansys Rocky's API:Solver used to introduce adsorption and desorption equations to allow multi-species transport between the CFD and DEM phases

Carbon capture simulation

- Use custom Rocky plugin to predict adsorption/desorption behavior with DEM-CFD coupled simulations

Particle Bed Generation in Rocky

Non-spherical particles are injected in the container to generate the fixed bed.

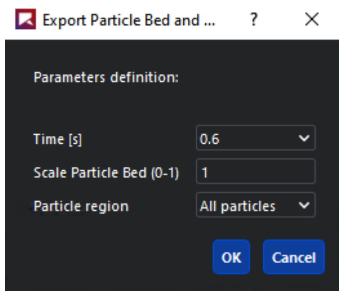
API:PrePost Scripting

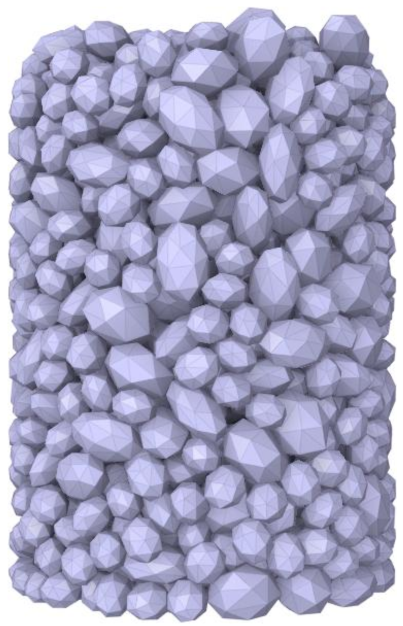
Particle info:

Shape
Position
Orientation
Size

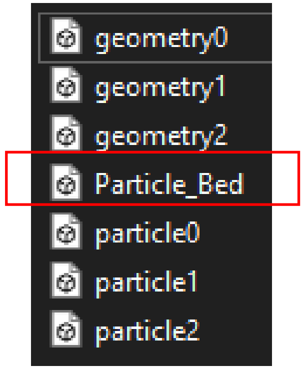
1) Export the .stl file of the particle bed;
2) Export the final state of the positions and orientations of the particles as .csv file

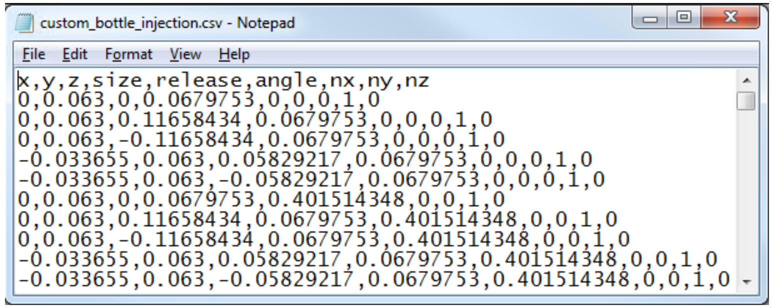
Ansys Rocky DEM: Realistic Packed Bed Generation Using Particle Filling





Particle bed .stl file



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x,y,z,size,release,angle,nx,ny,nz
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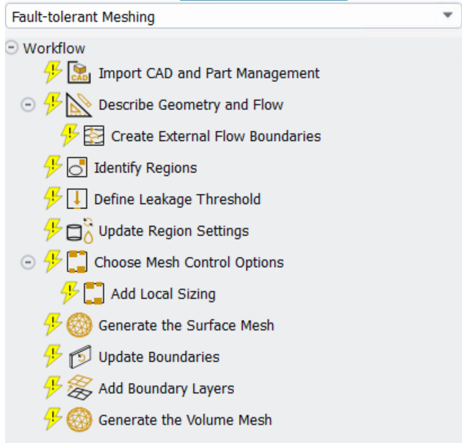
-0.033655,0.063,-0.05829217,0.0679753,0.401514348,0,0,1,0
```

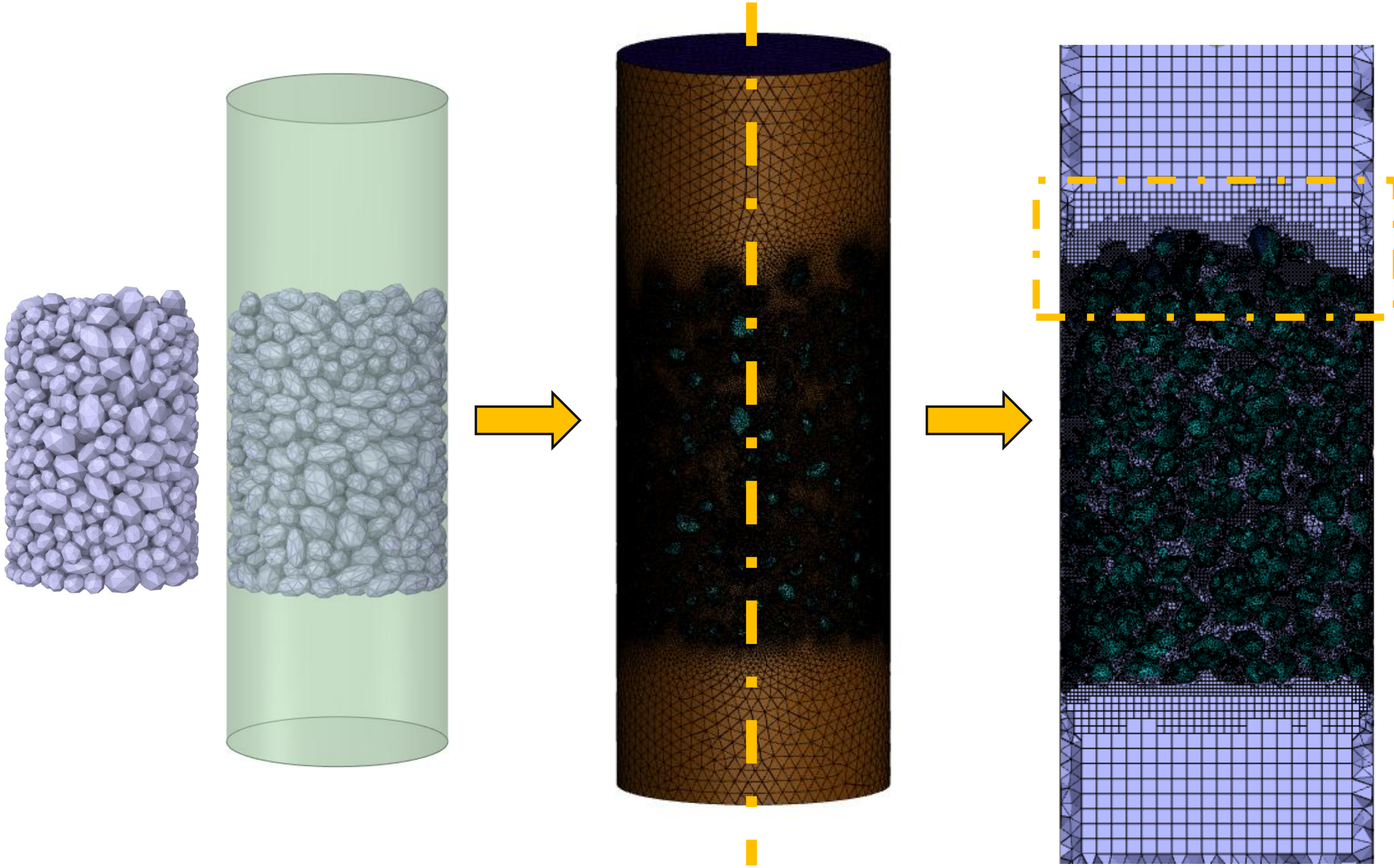
Example of a Particle Custom Inlet definition .csv file

The Custom Inlet .csv file is used further in the workflow

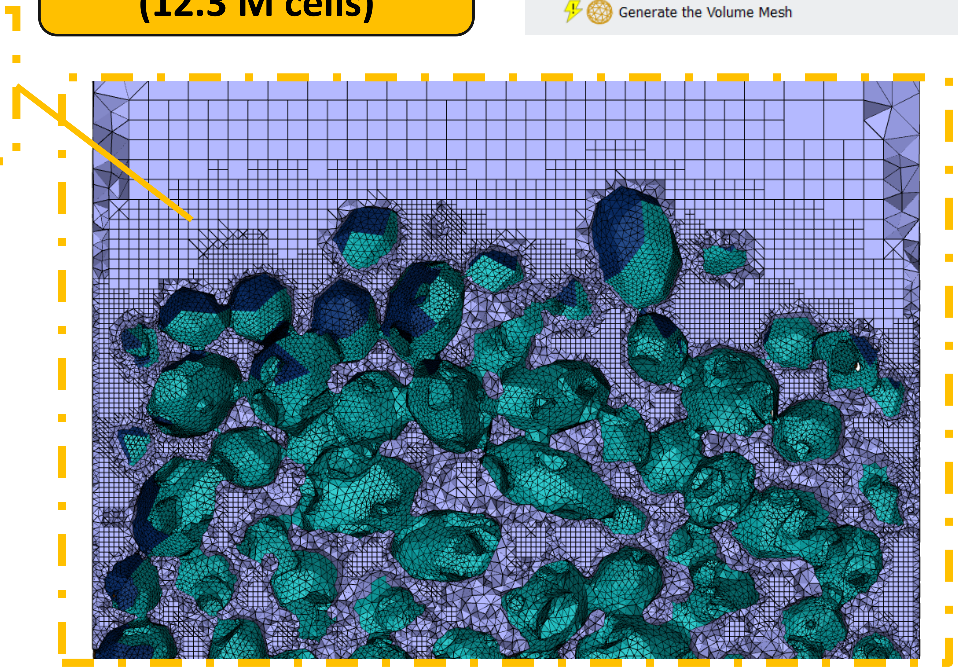
CFD Domain and Mesh Creation

- The particle bed geometry was placed in a fluid domain and consequently meshed:
- The meshing workflow of packed particle beds is based on **Fluent Meshing's "Fault tolerant meshing"** pre-defined workflow.





Hexcore mesh built with Fault-Tolerant Meshing Workflow (12.3 M cells)



Detail of a cut plane from the fluid domain around the particle bed

Reference Data Validation

CFD Setup

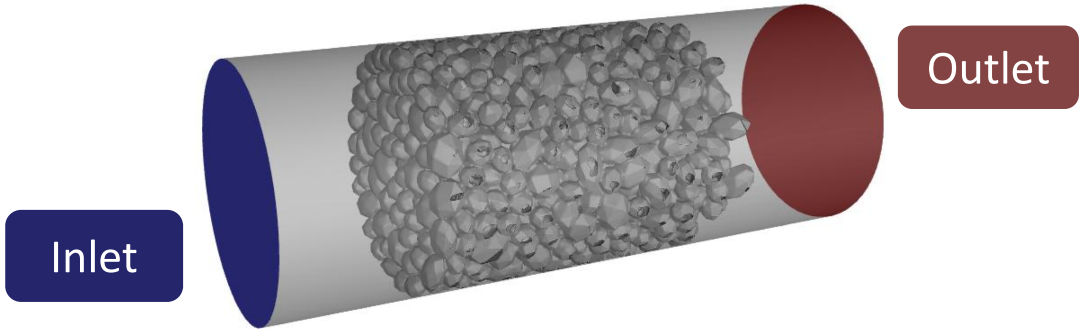
Velocity inlet (1, 2, 5 & 10 m/s)

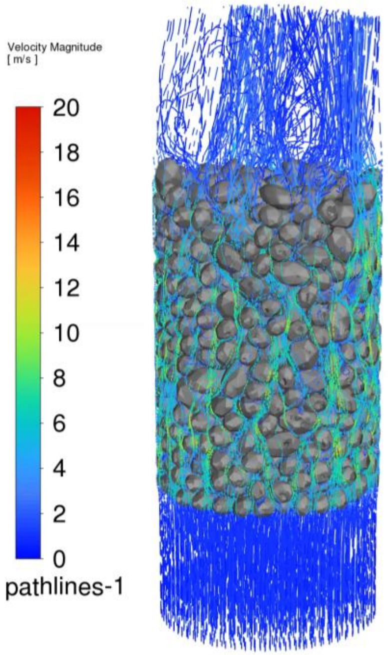
Pressure outlet (0 Pa Gauge Pressure)

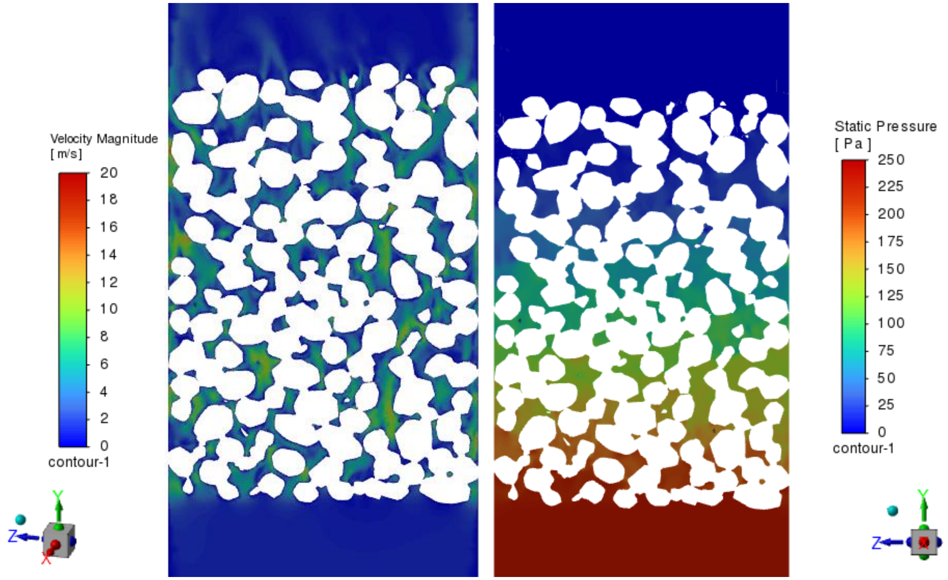
Mesh independence analysis

Pressure drop as comparison result

	Mesh size = 7.19 M cells	Mesh size = 12.3 M cells	Mesh size = 34 M cells
Inlet Velocity [m/s]		5	
Pressure drop [Pa]	6225.54	5653.76	5527.12
Diff. [%]	-	9%	2%







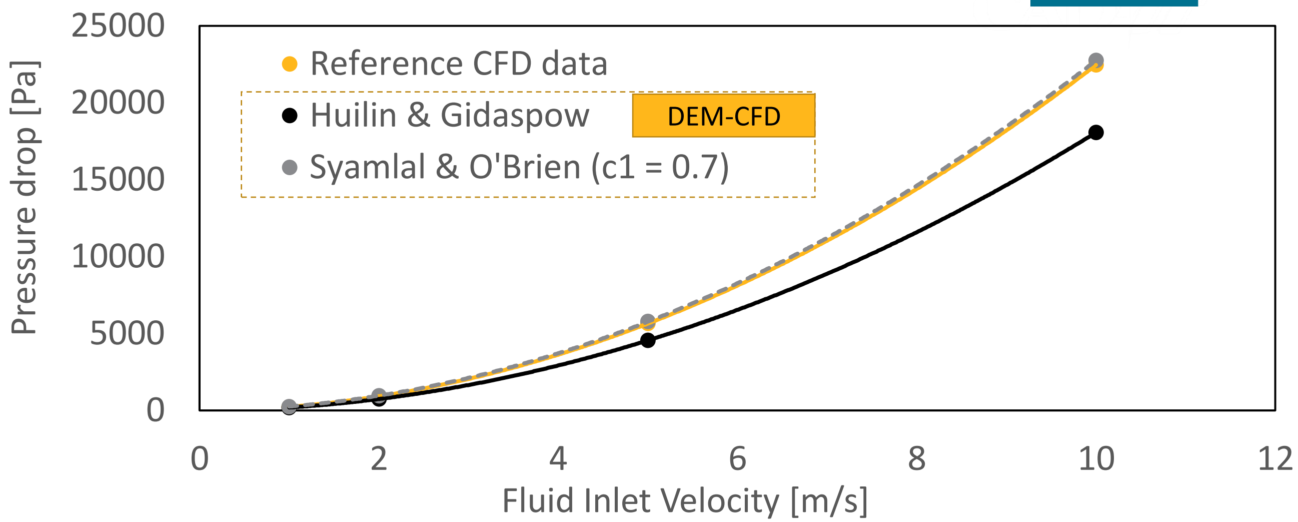
Post-processing for **standalone CFD simulation** (Fluid inlet velocity = 1 m/s)

DEM-CFD Setup and Calibration of Drag Laws

DEM-CFD Setup and calibration

DEM-CFD Drag law calibration

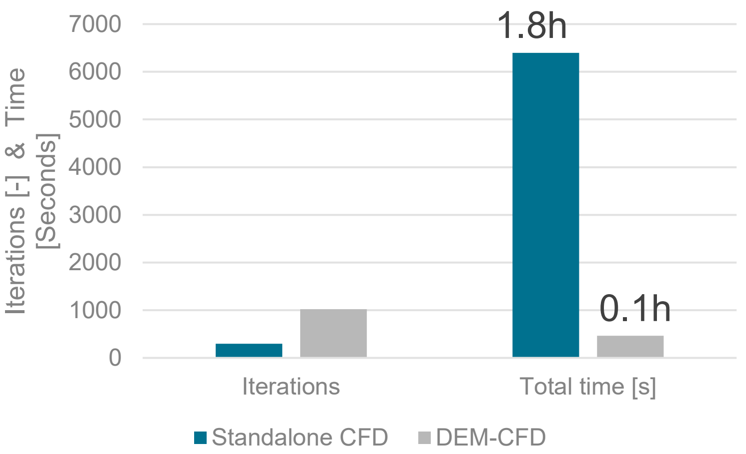
ΔP vs. Velocity curve as verification data

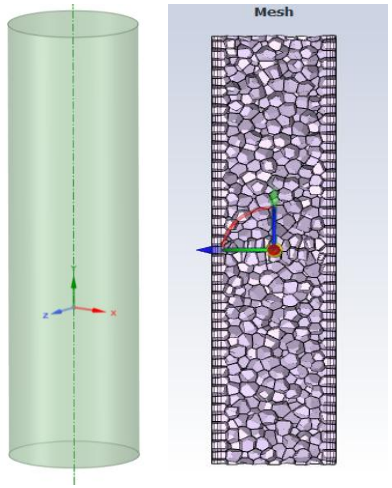


Mesh size:

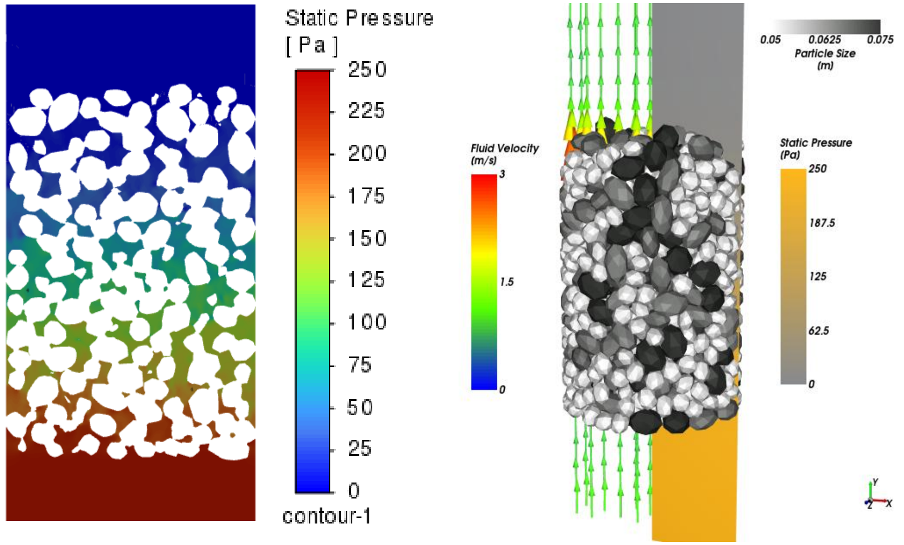
Standalone CFD:
12.3 M cells
Steady-state

DEM-CFD*:
1k cells
Transient





Geometry and Mesh for DEM-CFD coupling



Static Pressure in CFD and CFD–DEM Coupling, respectively.

Solver Customization

C++ API:Solver

Modules

User Parameters for the model!

Adsorption/Desorption rate

$$m^i = \alpha\left(n_f^i MW^i \frac{(P + R_{ref})V}{RT}\right)$$

The adsorption/desorption rate is assumed to be a constant fraction of the vapor species in the fluid phase. The liquid film solution is an ideal and the vapor phase is an ideal gas.

*This does not consider the impact of several species on the vapor-liquid equilibrium, the equilibrium is generated separately for each species.

Where:

i = Species (CO_2 and H_2O)

m = Mass (Vapour/Liquid Phase) [kg]

nf = Mole fraction [-]

MW = Molecular Weight [kg.kmol-1]

Alpha = Vapour/Liquid fraction [-]

P = Fluid Static Pressure [Pa]

Pref = Reference Pressure [Pa]

V = Cell Volume [m³]

R = Gas Constant [J.mol-1.K-1]

T = Fluid Temperature

Energy conservation

$$m_p C_p \frac{dT_p}{dt} = \sum \dot{q}_{cond} + \sum \dot{q}_{conv} + \sum \frac{dm^i}{dt} h^i_{ads}$$

Using the principle of energy conservation, the heat transfer rate to the particle considers contributions from conduction, convection, and heat produced during adsorption/desorption.

Where:

Tp = Particle Temperature [K]

h_ads/h_des = Heat of Adsorption/Desorption [J.mol-1]

Mass/Volume changes

$$\frac{dm_p}{dt} = \sum m^i C_{sw} \qquad \frac{dV_p}{dt} = \sum \frac{m^i}{\rho^i} C_{sw}$$

During adsorption/desorption, mass and volume changes follows these equations.

Where:

Mp = Particle mass [kg]

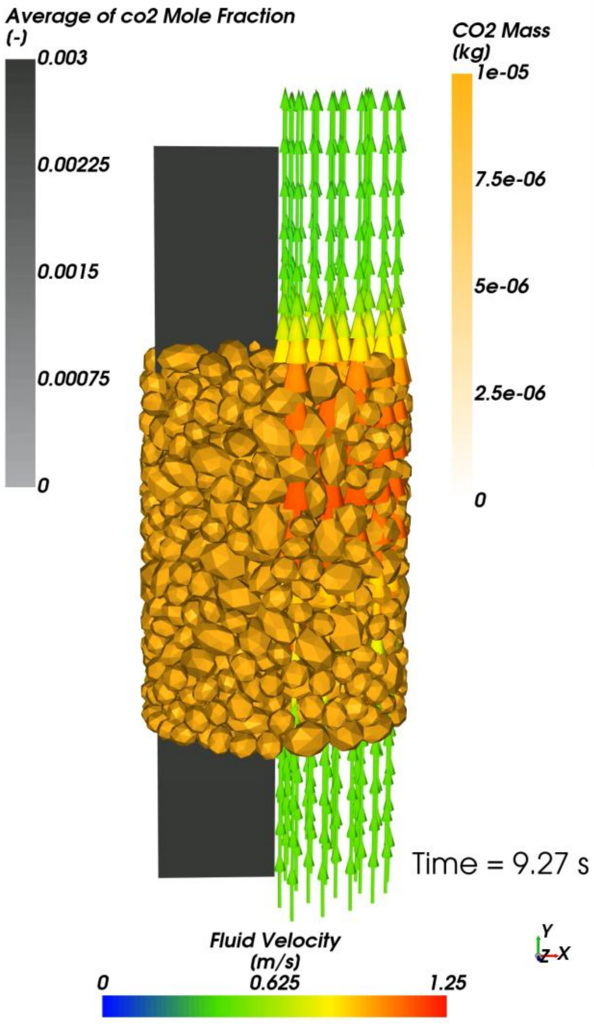
Vp = Particle volume [m³]

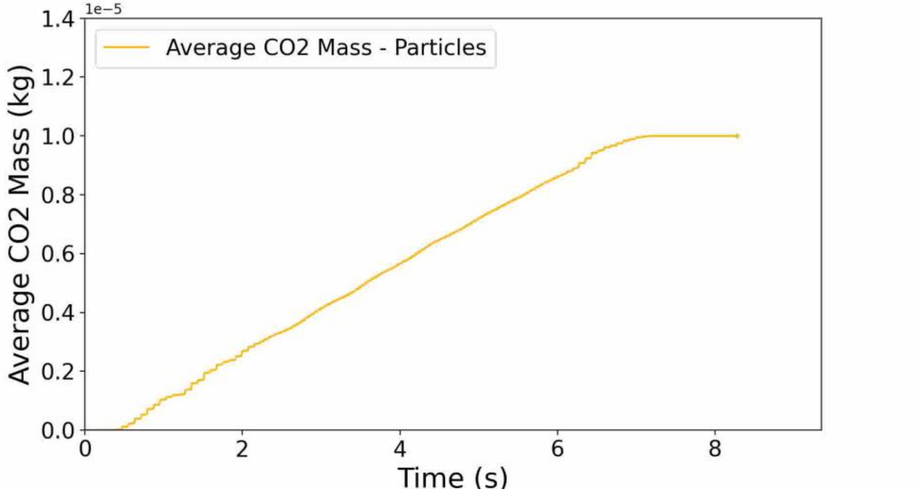
Csw/Cdsw = Swelling/Deswelling coefficient [-]

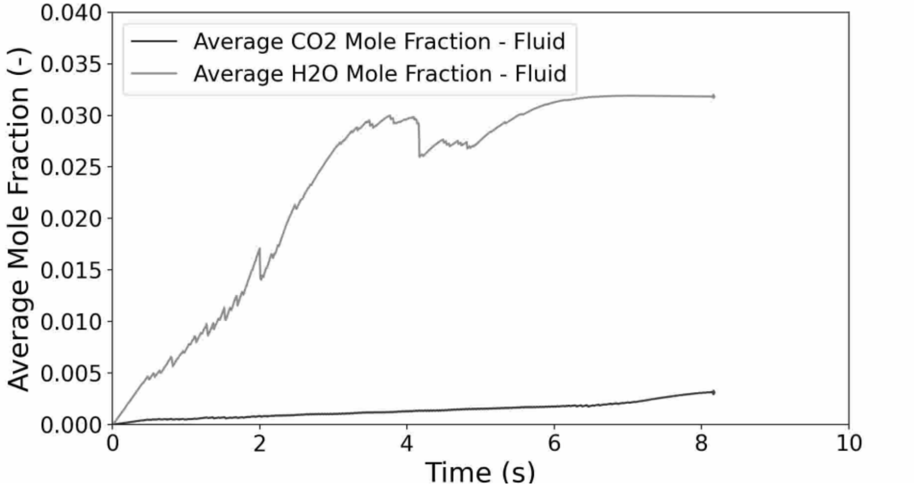
P = Density [kg/m³]

Adsorption Results: Carbon capture simulation

- With the **DEM-CFD** Adsorption simulation, we can observe:
  - Particle bed slowly saturates until user input is reached
  - Species-rich air begins to pass particle bed once particles are saturated







Outcome

- The DEM-CFD approach enables analyzing species concentration for each particle in the domain, as well as volume and mass change of the particles.
- Complex designs can be evaluated to find which ones have better adsorption or desorption.
- Find the particle shape and size distribution that provides the desired pressure drop and porosity conditions.

THANK YOU

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