

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

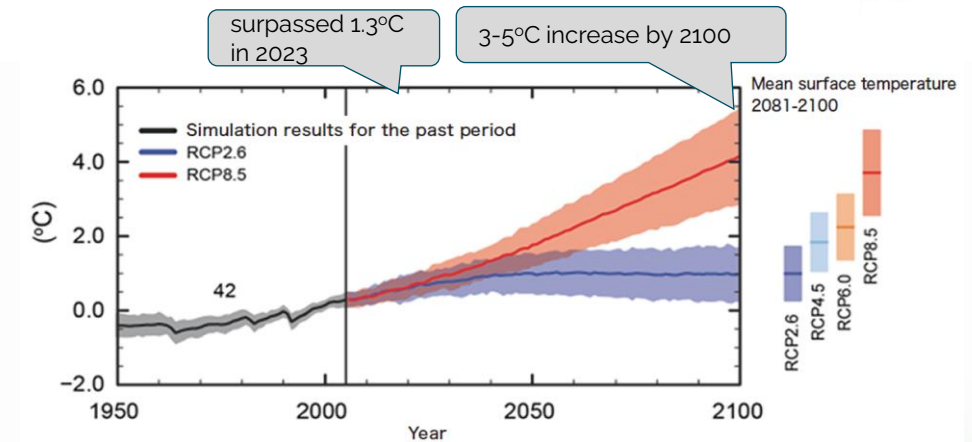
Supitcha S.

Asst. Technical Manager
CADIT (Thailand) Co., Ltd.

Global Decarbonization Trends: Low-Carbon Energy Solutions



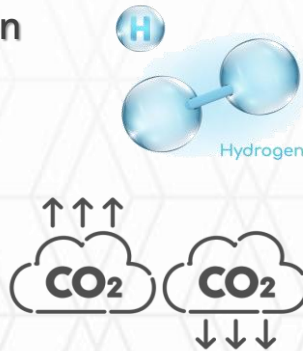
- CO₂ emissions are the primary driver of global climate change
- **Paris agreement:** CO₂ emission reduction
 - Keep temperature rise below 2°C, preferably 1.5°C
 - Already above 1.2°C, on track to pass 1.5°C by 2030
- The **energy sector** is a source of around **75% of GHG** today
- Need for a cleaner energy system



Global surface temperature continue to increase

- 50% of CO₂ 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

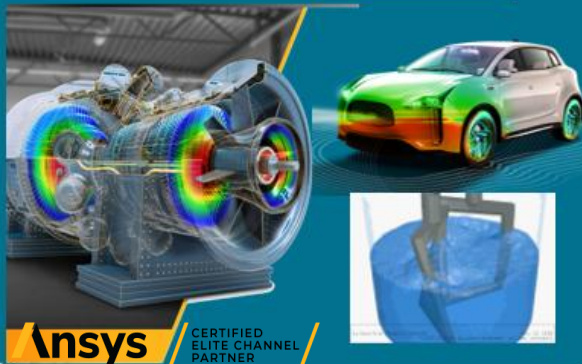
Vision

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



Increase capacity in polymerization reactors

Application Example

Objective:

- Obtain how well the raw materials in the reactor were mixed
- Design the new polymerization reactors to double capacity with concerning about keeping production yield and product properties

Increase Biomass Boiler Capacity

Application Example

Objective: Biomass boiler retrofit to increase capacity

Anslys Solution

After retrcom temj time Valu

Enhance Research Quality and Productivity

Application Example

Benefits:

- PTT Global Chemical gained benefit from using ANSYS by several factors, mainly in
- Process improvement and troubleshooting
- Product design and development
- Save cost and time (research, trial, maintenance)

Quality:

- Prevent shutdown situation by forecasting cause of problem
- Increase product capacity by increasing production efficiency
- Gain suitable/optimize design for new product and process in terms of engineering

Cost:

- Reduced design/prototype cost
- Reduced testing cost
- Reduced redesigning raw material usage

Time:

- Reduced testing time
- Reduced repeatability and optimization time
- Reduced research and engineering time
- Reduced time to launch new performing products

"ANSYS is the best CAE tool ever because of the ease of use, full functionalities in Structural and CFD analysis as well as couple analysis (FSI). It helps us to enhance our research quality and productivity to enable us to make correct decisions understand better and analyze faster"

Mr. Nattapong Tarapooms,
Researcher, R&D - Scale up and Process Technology, Downstream Innovation

2 Improving Reliability & Affordability



Understand Cause of Failure of Burner Diffuser

Application Example

Objective: Optimize burner for diffuser overheat solving in waste heat recovery unit

Challenges

- Finding the solution and the cause of the problem to reduce production loss
- To obtain an accurate result of the temperature distribution inside the burner

Understand Cause of Chimney Trays Collapse

Application Example

Objective: To analyses the unreachable unit

Challenges

- Solving of Volume of Fluid (VOF) model in a complex geometry accurately
- Post-processing for complex geometry/large file smoothly
- Providing the solution (animation) effectively to provide strong evidence for maintenance implication

Understand Structural Behavior of Expansion Joint Misalignment

Application Example

Objective:

- Misalignment from assembly lead to exceed deformation and unexpected failure. The geometry nonlinearity which involves material nonlinearity are difficult to find the maximum stress accurately and reliable.

ANSYS Solution

- Perform non-linear material and large deformation static structural analysis of the expansion joint under defined displacement to investigate the stress and deformation

Value of Simulation

- Understand the structural behavior due to apply load and boundary conditions in a better view which help effectively communicate with our staffs to point out the weakest position and the prior part to be maintenance.

"Our Maintenance department deals with monitored / preventive maintenance to ensure reliability and integrity of equipment through the applicat of condition. So we need the precise tool that can predict the failure of the operating equipment. ANSYS Mechanical module has been used to analyze the complex problems which help us to understand the root cause of failure and to correct prevent it accurately. Moreover, technical support from CAD-IT is an important part of our team success. Not just help solving challenging tasks within short time period but also be a good consultant"

Mr. Pisanu Punyaporn,
Maintenance Engineer Manager

Mr. Nonthawat Tianwong,
Mechanical Engineer

3 Maturing Low Carbon Solutions



Predicting Wind Power

Engineering Goals

- Noise, energy prediction, unplanned downtime, and maintenance all pose significant issues during wind farm siting and operations

Solution

- Anslys multiphysics analysis generated an automated wind farm simulation workflow to assess site output and efficiency
- Digital twins of wind turbines offered predictive analysis

Customer Goals

- Achieve highly efficient electrolyzer design
- Ensure better partial load behavior
- Increase the power density of the stacks
- Ensure sufficient electrical conduction to the reaction points and to dissipate the heat generated during the electrolysis

Solution

- Intuitive, flexible, and robust meshing for complex

Hydrogen Production: Water Electrolysis

PEM Electrolyzer

PEM Electrolyzer: γ_{H_2} and γ_{O_2}

Hydrogen fraction in an electrolysis cell at different flow rates with straight parallel channels.

"These results from Ansys tools will contribute to the future manufacture of better-performing, lower-cost, energy-efficient and durable PEM electrolyzers"

Ernesto Amorim Vera, Research and Development Engineer, Centro Nacional del Hidrogeno (CNH2)

Post-Combustion Carbon Capture – Chemical Absorption

- The process flow diagram for CO₂ absorption and the geometry considered for investigation are shown below:

- 2 fluid Eulerian model; Billet Drag
- Chemical reaction - Heterogeneous
- Heat transfer - Porous media - Packed bed

$CO_2 + 2RNH_2 \rightarrow RNHCOO^- + RNH_3^+$

$log(k) = 10.99 - 2152/T$

CO₂ mass fraction at outlet (1.6% predicted) (1.2% measured)

Flue gas out

Liquid Zone

Porous Zone

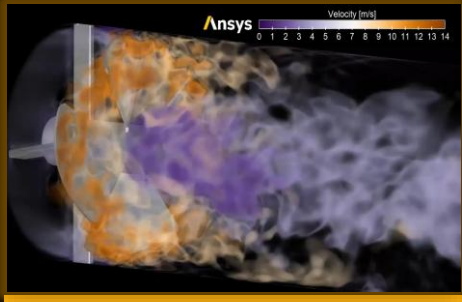
Metal Raschig rings; randomly packed

Flue gas (air + CO₂)

Source: P. Rittigkowsky, D. Auerdyck, Amine based CO₂ capture – CFD simulation of absorber, absorber, Absorber Mechanical Engineering, 2011, 2022-2024



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

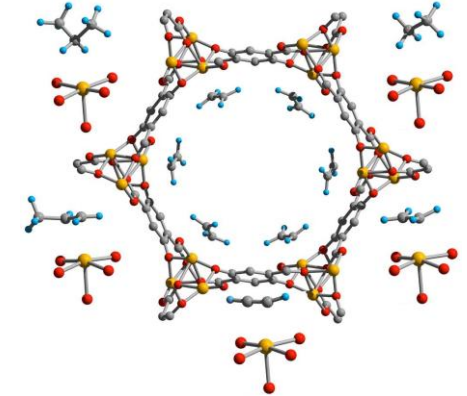


- Model Based System Eng.
- Requirements & architecture Connections
- Safety, security, & software
- Digital twins
- Simulation process & data management
- Mission engineering

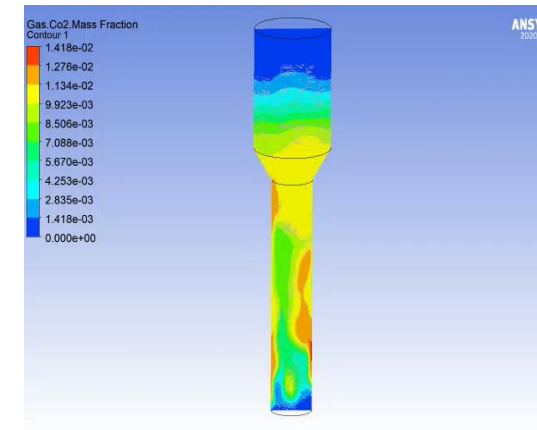
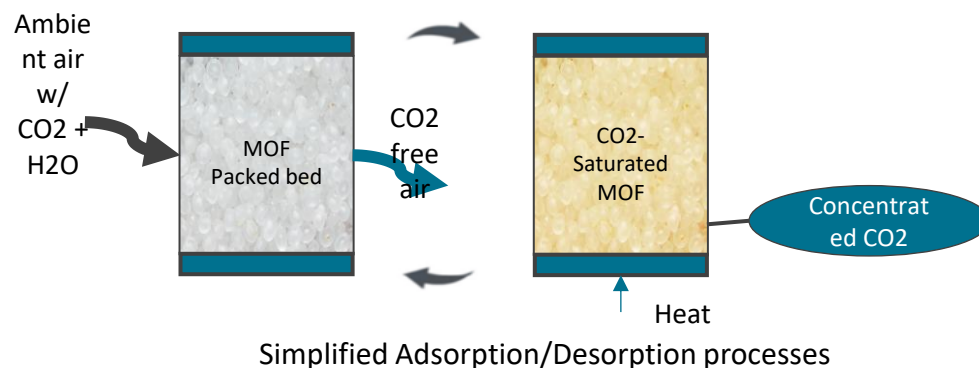
The Digital Transformation Will Accelerate Pillars #1, #2 & #3 and Drive Scaling ...

Background: Carbon Capture in Particle-Bed Reactors

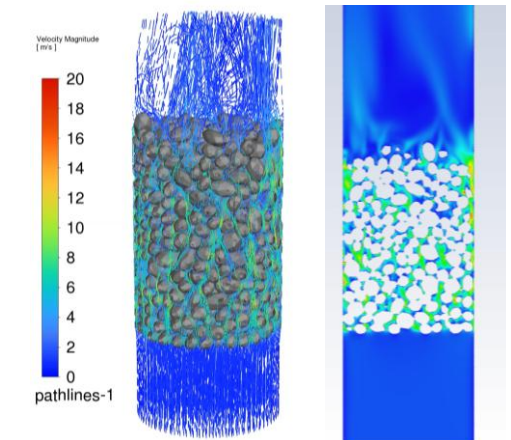
- Particle-bed reactors are widely used in chemical process industries, such as for the process of capturing carbon dioxide.
- Carbon capture using **particle-bed reactors** involves passing **CO₂-containing gas (flue gas)** through a bed of **solid particles (sorbents)**. **MOF materials** are commonly 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.



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



Solution for CO₂ distribution in dense fluidized bed for FCC regenerator

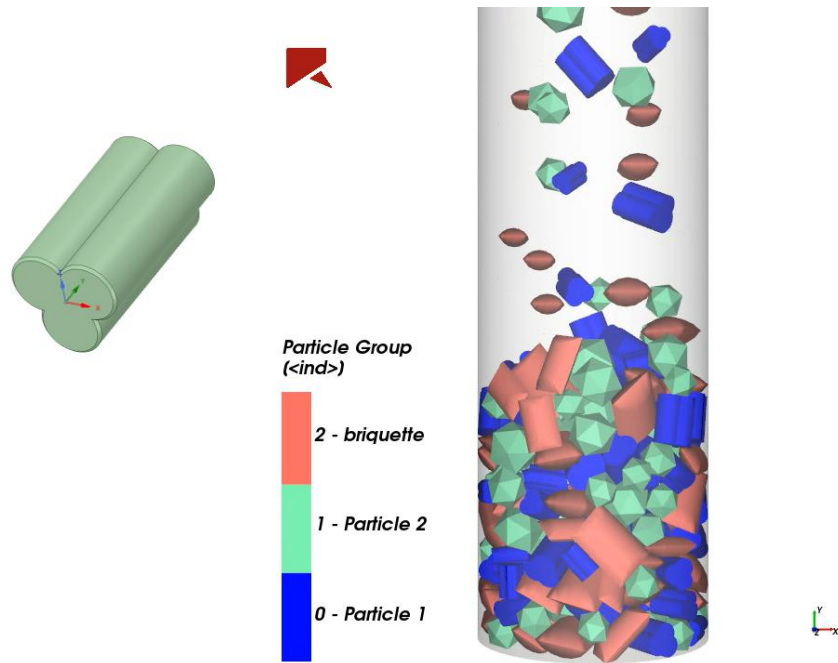


Fixed Bed Reactor

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

/ Ansys Rocky (DEM)

Rocky enables the creation of porous media made of particle beds

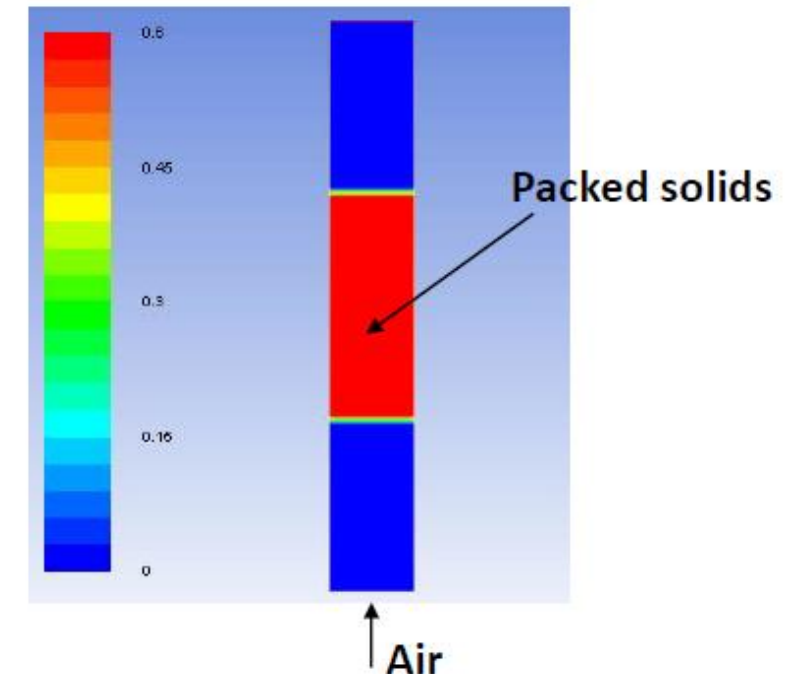


MICROSCALE (Particle-resolved): Volume Fraction, Momentum and Heat exchange terms



/ Ansys Fluent (CFD)

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



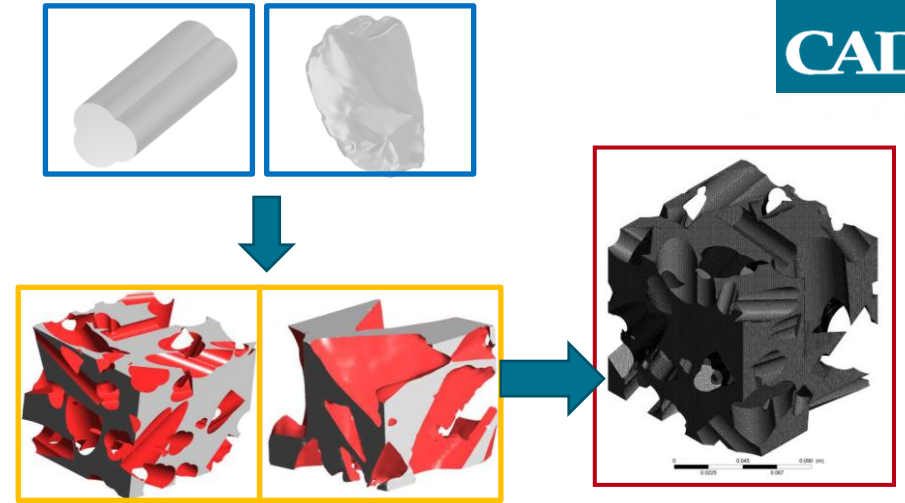
MACROSCALE (Fluid-resolved): Two-fluid averaged equation approach : Fluid Velocity and Pressure Fields



Complexity & Simulation Challenges

Engineering Goals

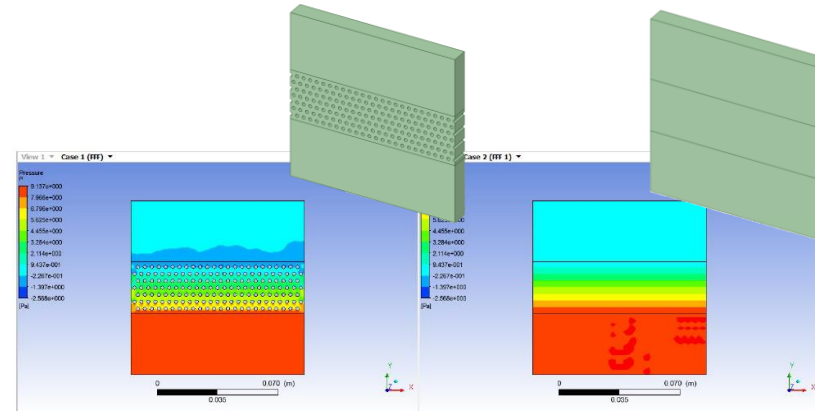
- Evaluate the performance of Metal-Organic Frameworks (MOFs) on adsorption of carbon dioxide from ambient air and desorption processes.
- Predict particle bed porosity and permeability.
- Evaluate effects of particle swelling/deswelling on pressure drop and porosity.



Complexity & Simulation Challenges

Devices are very complex

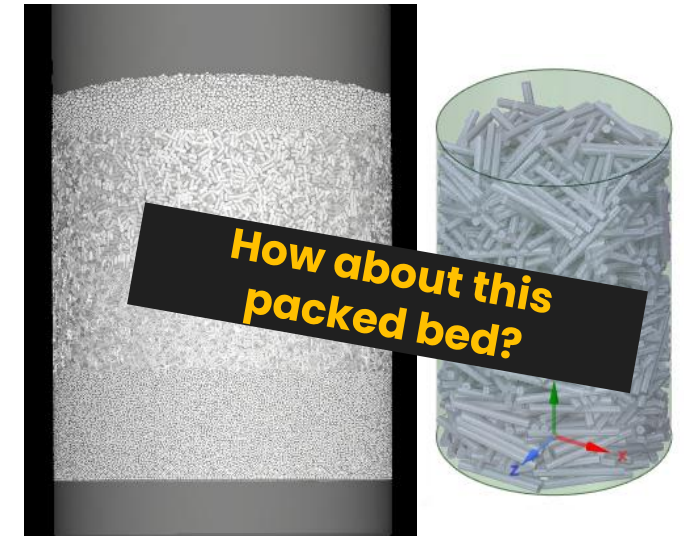
- Scale bridging (particle → reactor)
- Complex geometry: how to represent the porosity and permeability properties of particle beds
- Complex mesh
- Complex boundary conditions
- Complex physics: Turbulence; Multiphase flow (gas–solid interaction); Chemistry



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

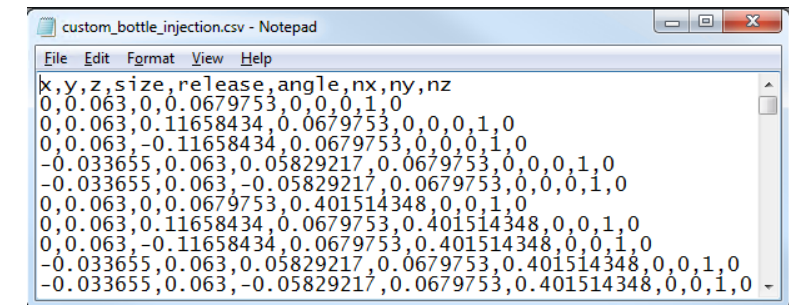
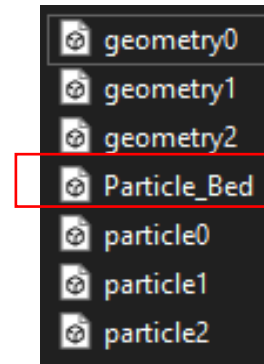
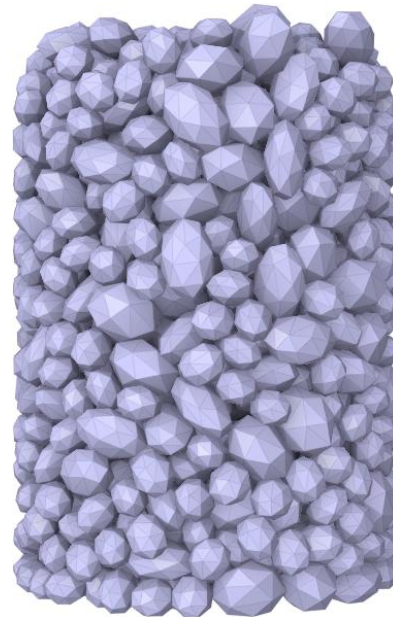
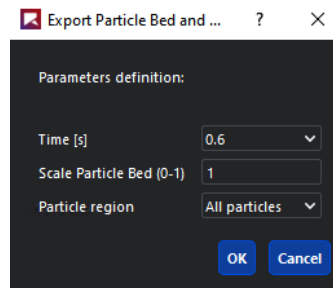
Particle Bed Generation in Rocky

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



Example of a Particle Custom Inlet definition .csv file

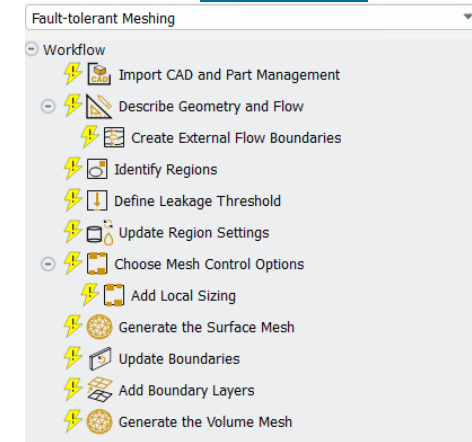
The Custom Inlet .csv file is used further in the workflow

Particle bed .stl file

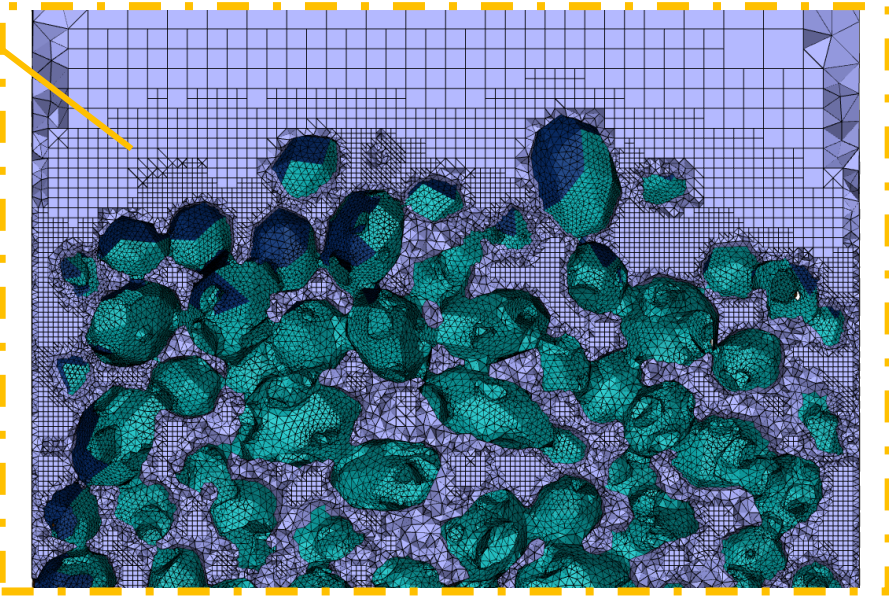
Ansys Rocky DEM: Realistic
Packed Bed Generation Using
Particle Filling

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



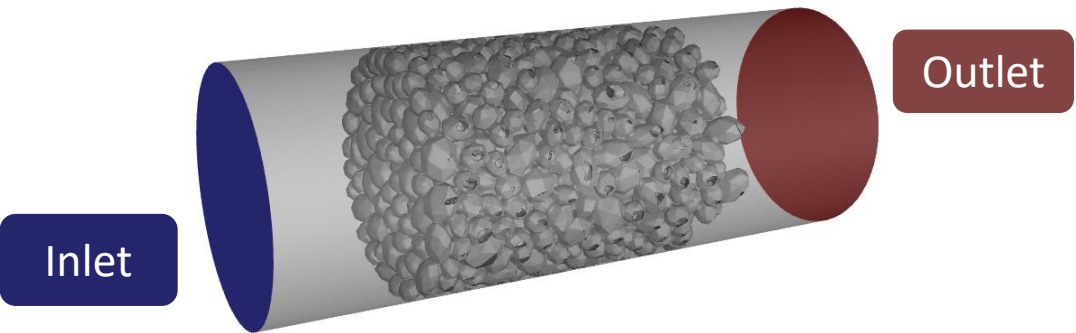
CFD Setup

Velocity inlet (1, 2, 5 & 10 m/s)
Pressure outlet (0 Pa Gauge Pressure)

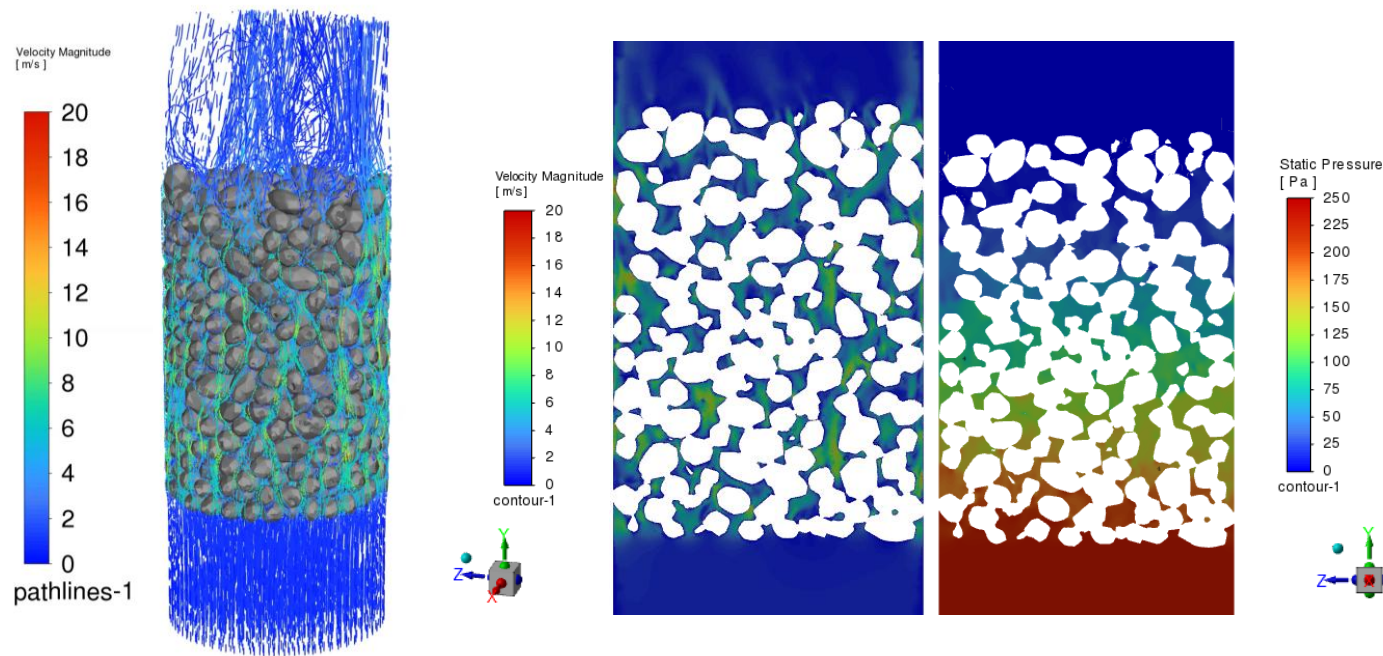


Mesh independence analysis

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%



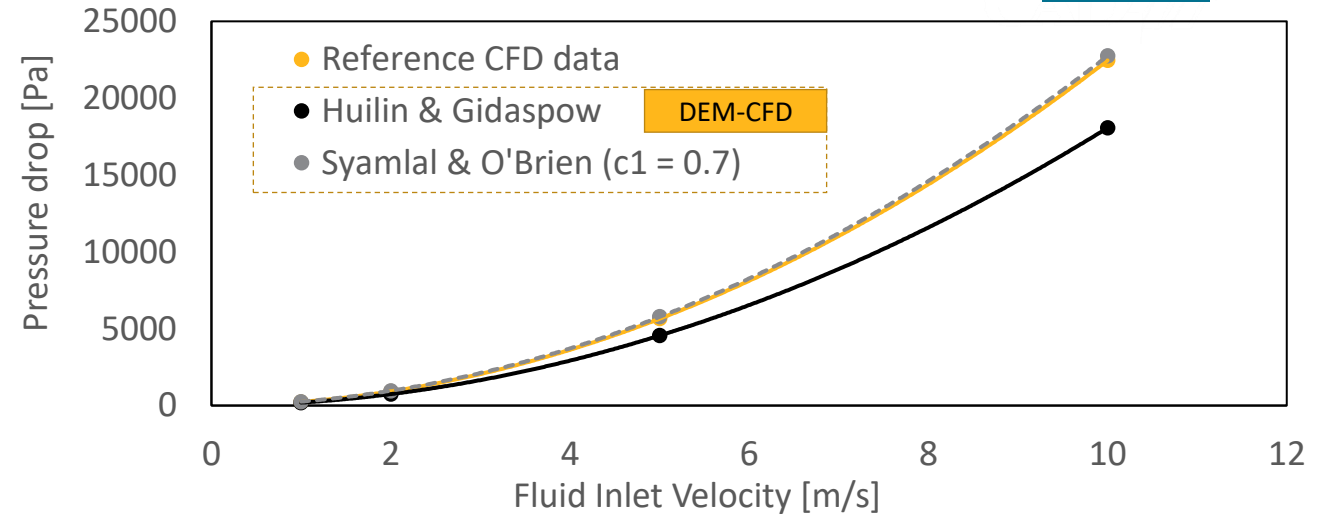
Post-processing for standalone CFD simulation (Fluid inlet velocity = 1 m/s)

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



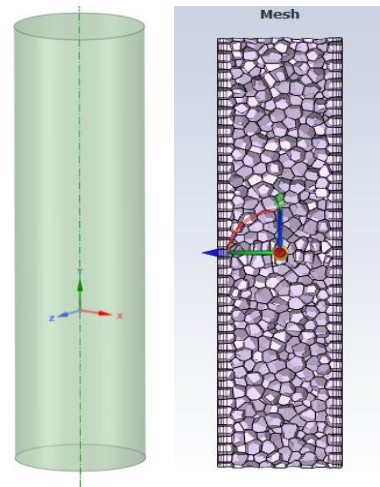
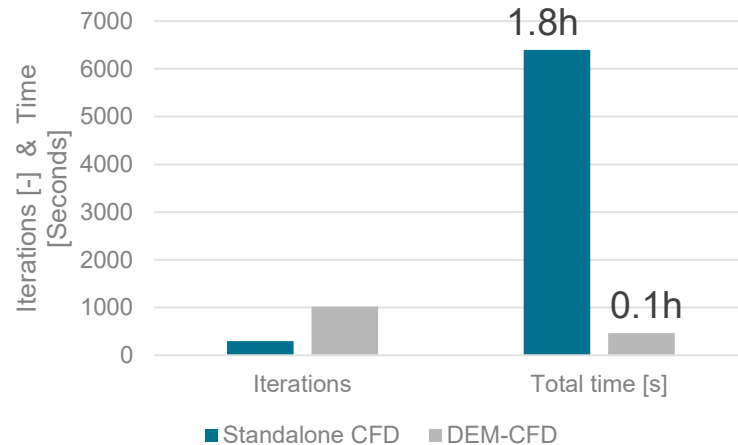
Mesh size:

Standalone CFD:
12.3 M cells

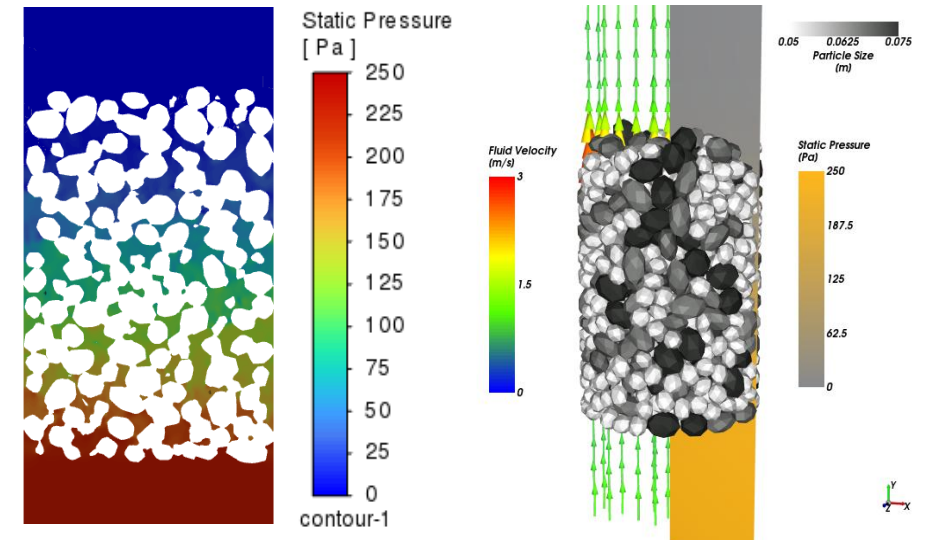
Steady-state

DEM-CFD*:
1k cells

Transient



Geometry and Mesh for DEM-CFD coupling



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



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 (CO2 and H2O)
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

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

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

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

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

Where:

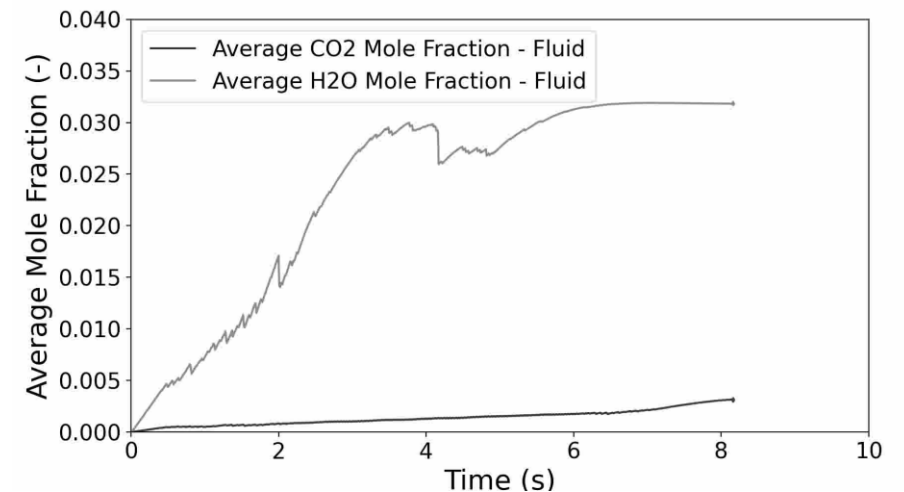
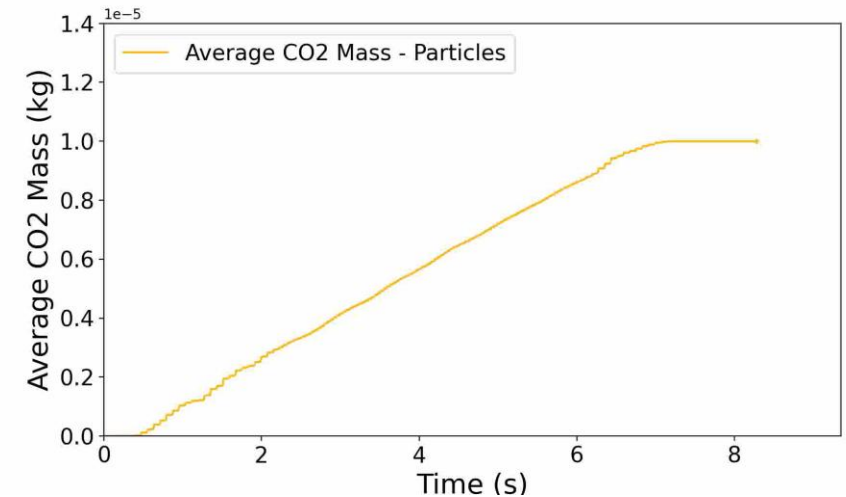
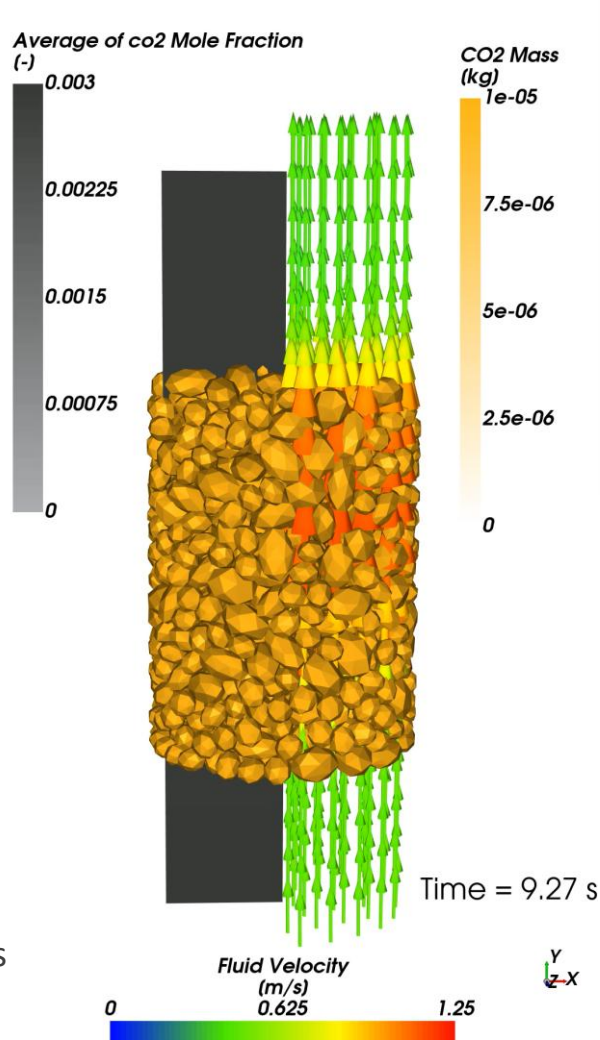
Mp = Particle mass [kg]
Vp = Particle volume [m³]
Csw/Cdsw = Swelling/Deswelling coefficient [-]
P = Density [kg/m³]

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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