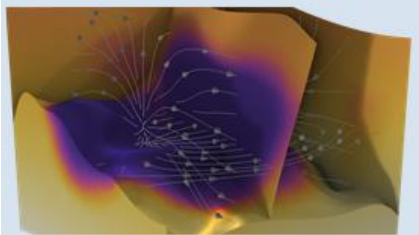


Heat and Moisture Transport in Porous Media

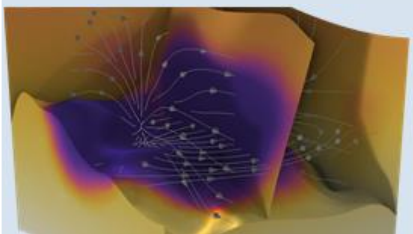
Nancy Bannach
COMSOL

Diversity of Porous Media

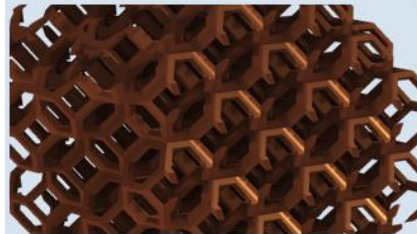


Geothermal Reservoirs

Diversity of Porous Media

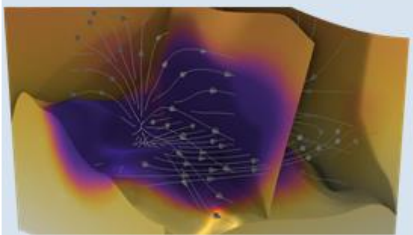


Geothermal Reservoirs

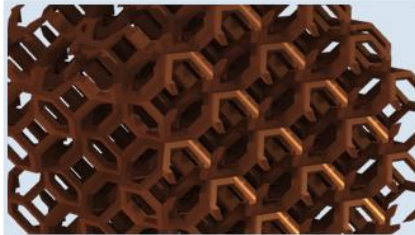


Material Science

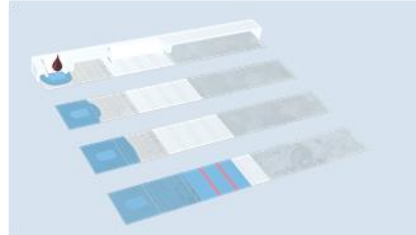
Diversity of Porous Media



Geothermal Reservoirs

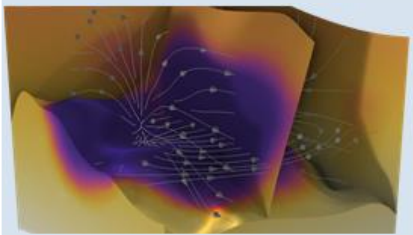


Material Science

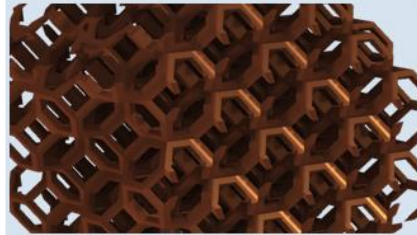


Healthcare Applications

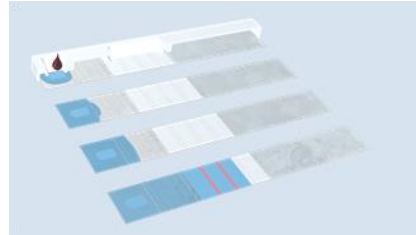
Diversity of Porous Media



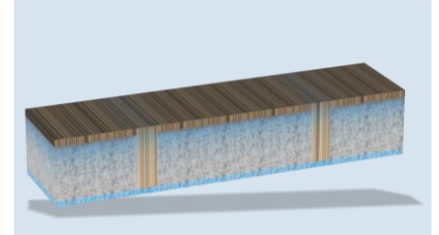
Geothermal Reservoirs



Material Science

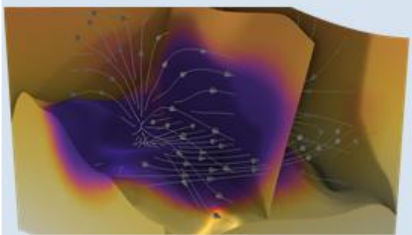


Healthcare Applications

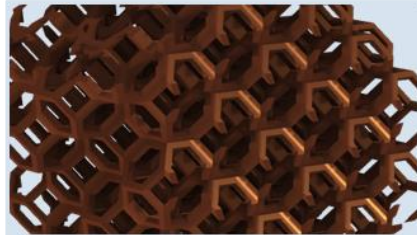


Building & Construction

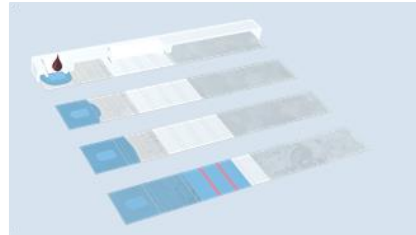
Diversity of Porous Media



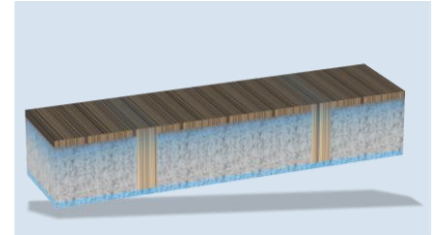
Geothermal Reservoirs



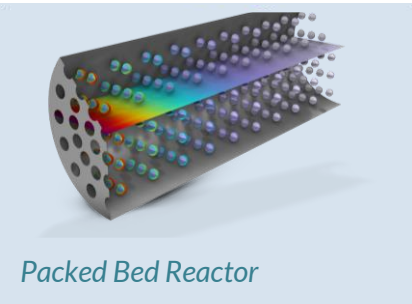
Material Science



Healthcare Applications

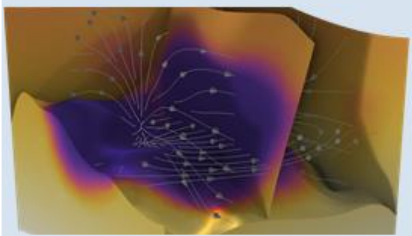


Building & Construction

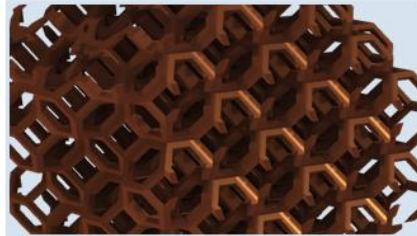


Packed Bed Reactor

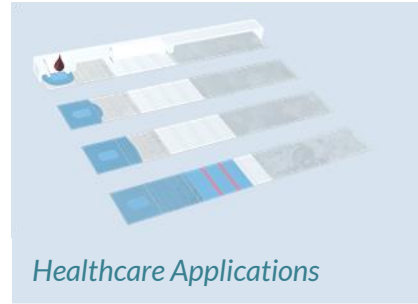
Diversity of Porous Media



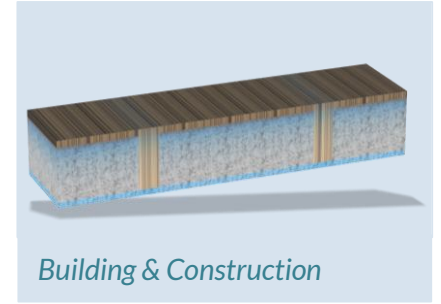
Geothermal Reservoirs



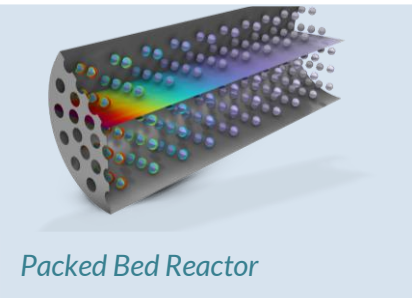
Material Science



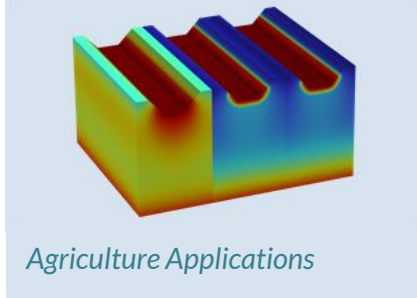
Healthcare Applications



Building & Construction

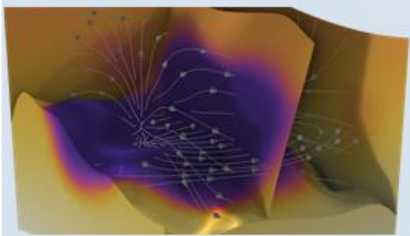


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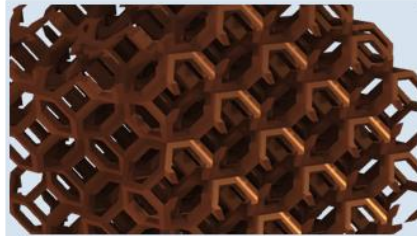


Agriculture Applications

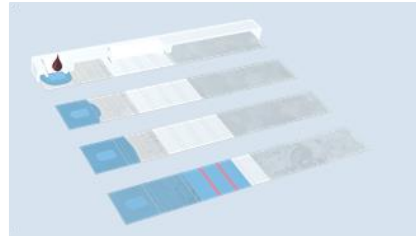
Diversity of Porous Media



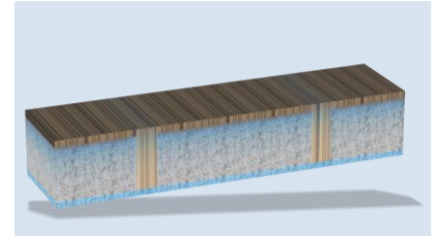
Geothermal Reservoirs



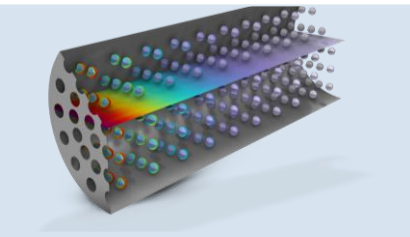
Material Science



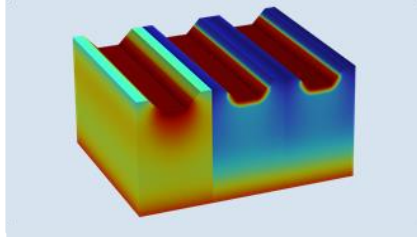
Healthcare Applications



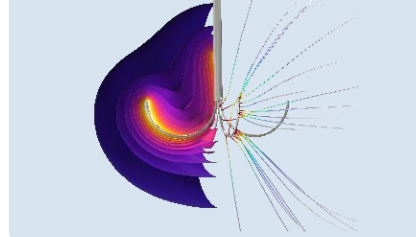
Building & Construction



Packed Bed Reactor

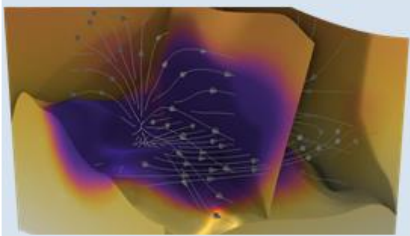


Agriculture Applications

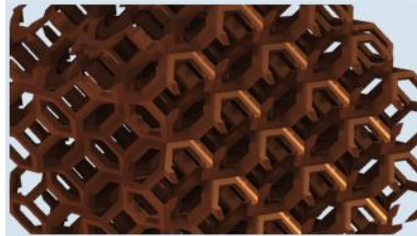


Biological Tissue

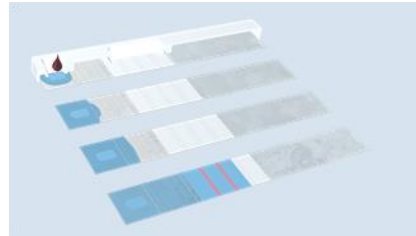
Diversity of Porous Media



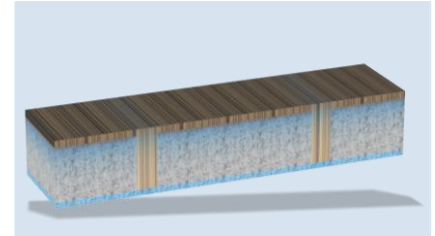
Geothermal Reservoirs



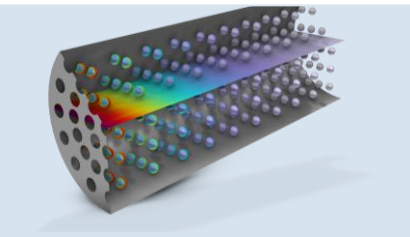
Material Science



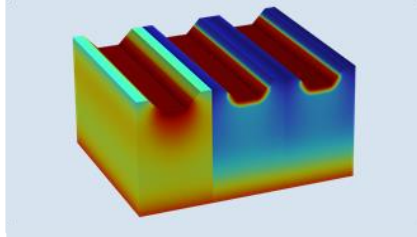
Healthcare Applications



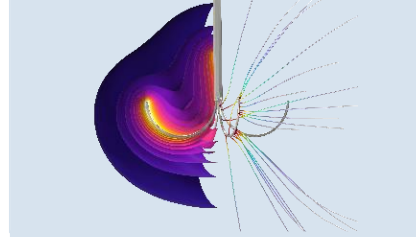
Building & Construction



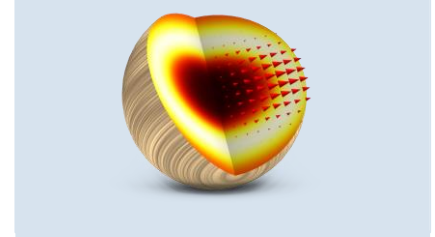
Packed Bed Reactor



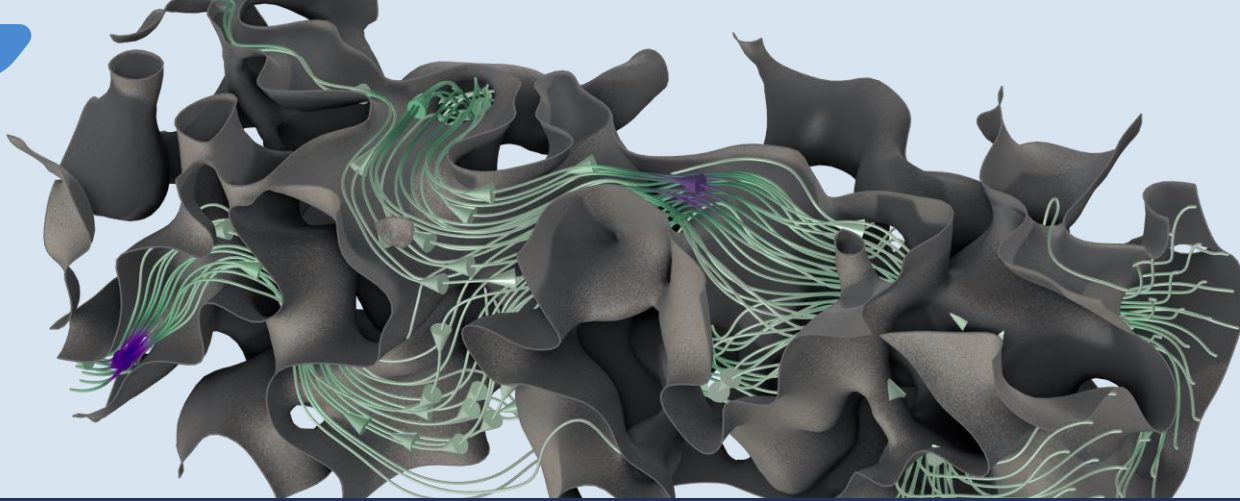
Agriculture Applications



Biological Tissue



Wood & Paper industry



From Pore-Scale Modeling...

Definition

Explores fluid behavior at the pore level, crucial for understanding capillary action and complex porous media dynamics

Applications

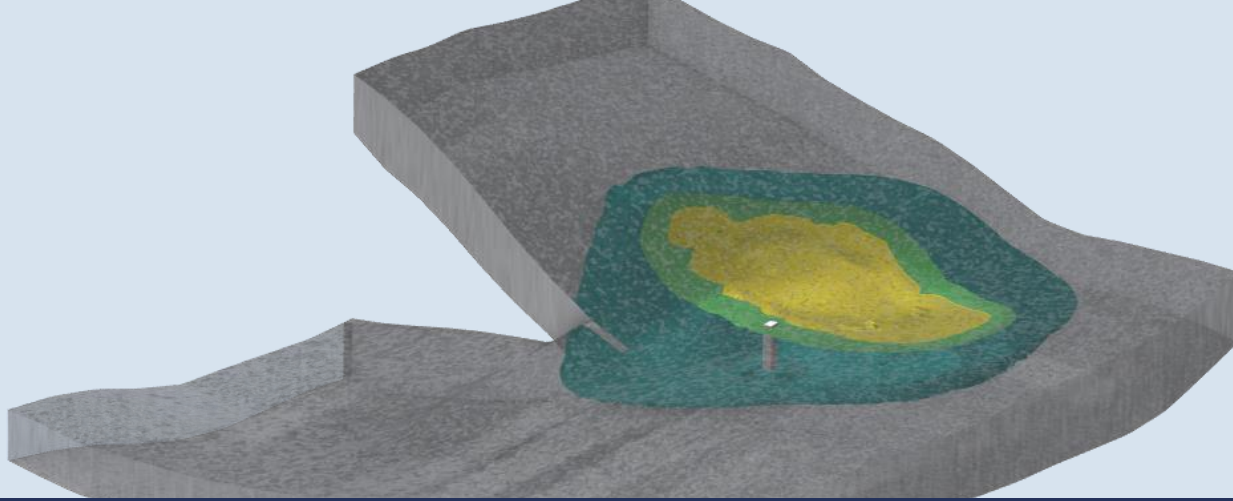
Predicting permeability, understanding multiphase flow, and simulating fluid behavior in biological tissues

Considerations

Fluid properties, boundary conditions, and surface interactions are essential factors for accurate microscopic modeling

Challenges

Intensive computational requirements and the necessity for precise pore geometry representation, crucial for achieving accurate simulations



...to Field-Scale Modeling

Definition

Modeling of large-scale applications with complex fluid dynamics and transport processes in heterogeneous environments

Applications

Optimizing resource extraction strategies, assessing environmental impacts, and informing sustainable engineering practices

Considerations

Fluid properties, boundary conditions, and surface interactions are essential for realistic simulations

Challenges

Precise representation of heterogeneous structures, integration of datasets, and the complex dynamics of chemical processes and materials

COMSOL MULTIPHYSICS®

The platform product for simulating real-world designs, devices, and processes. One user interface for all engineering applications.

- MODEL BUILDER: Combine physics phenomena in one model
- APPLICATION BUILDER: Build simulation apps from models
- MODEL MANAGER: Collaborate and organize models and apps

COMSOL Compiler™

Compile simulation apps into executable files. Run them freely on any computer.

COMSOL Server™

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- Ray Optics Module
- Plasma Module
- Semiconductor Module

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- CFD Module
 - Mixer Module
- Polymer Flow Module
- Microfluidics Module
- Porous Media Flow Module
- Subsurface Flow Module
- Pipe Flow Module
- Molecular Flow Module
- Metal Processing Module
- Heat Transfer Module

STRUCTURAL & ACOUSTICS

- Structural Mechanics Module
 - Nonlinear Structural Materials Module
 - Composite Materials Module
 - Geomechanics Module
 - Fatigue Module
 - Rotordynamics Module
- Multibody Dynamics Module
- MEMS Module
- Acoustics Module

CHEMICAL

- Chemical Reaction Engineering Module
- Battery Design Module
- Fuel Cell & Electrolyzer Module
- Electrodeposition Module
- Corrosion Module
- Electrochemistry Module

MULTIPURPOSE

- Optimization Module
- Uncertainty Quantification Module
- Material Library
- Particle Tracing Module
- Liquid & Gas Properties Module

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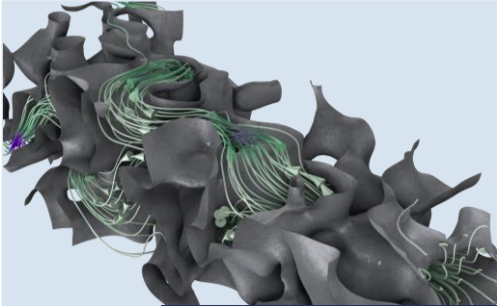
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Fluid Flow in Porous Media

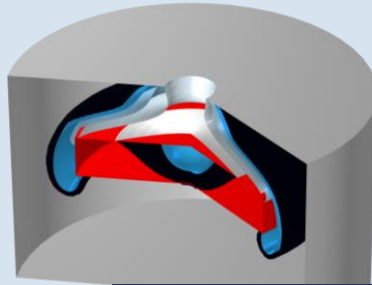


Single Phase Flow

Laminar or Creeping flow

Darcy's law, Richards' Equation

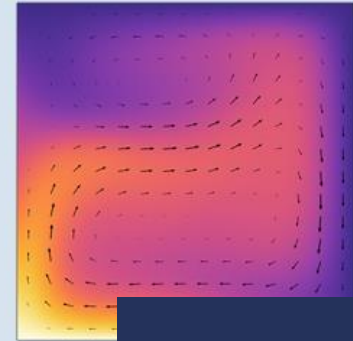
Brinkman equations
(Laminar, Turbulent)



Multiphase Flow

Multiphase transport

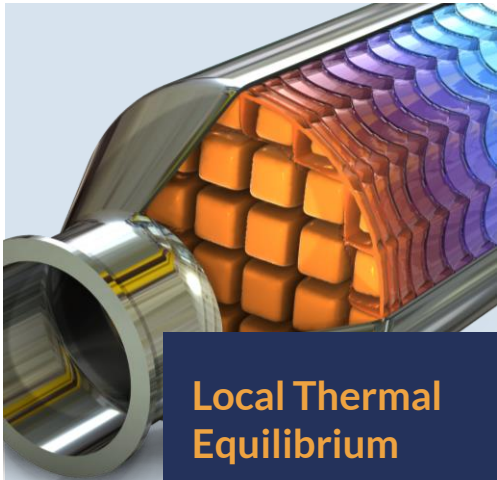
Front tracking with Level-set Brinkman



Nonisothermal Flow

Predefined coupling of Brinkman equations and heat transfer in porous media

Heat Transfer in Porous Media



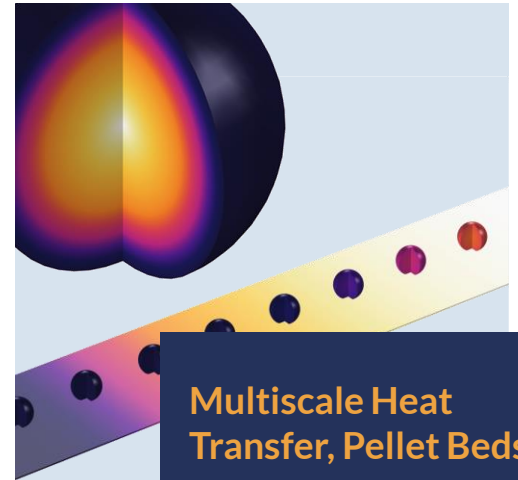
Local Thermal Equilibrium

Homogenized porous media; predefined models for effective thermal conductivity



Local Thermal Nonequilibrium

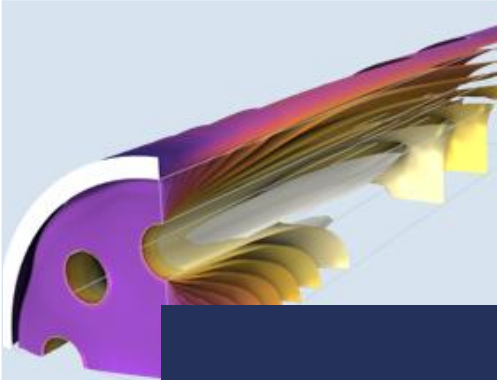
Two-temperature model for porous media where the fluid and solid temperatures differ



Multiscale Heat Transfer, Pellet Beds

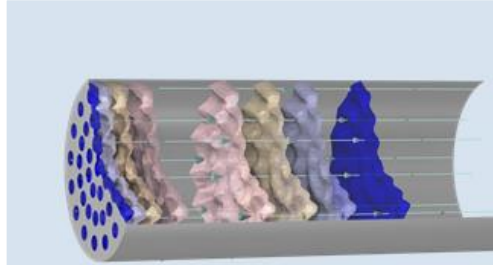
Models the temperature in the fluid and the temperature distribution in the pellets at every point

Transport in Porous Media



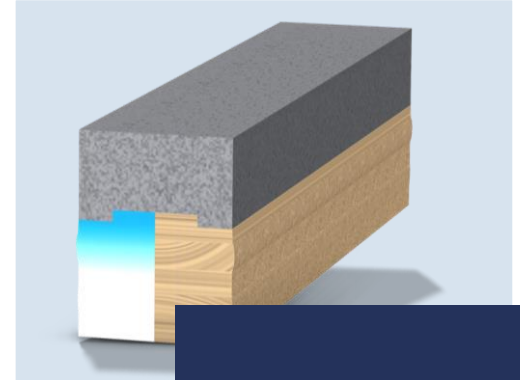
Solute

Diffusion, conduction, and dispersion models
Adsorption isotherms
Volatilization



Multicomponent

Multicomponent transport in liquids and gases
Maxwell–Stefan diffusion, Mixture average, Knudsen Diffusion



Moisture

Liquid water and moist air in equilibrium.
Vapor diffusion and convection in moist air
Convection and capillary flow in the liquid phase.

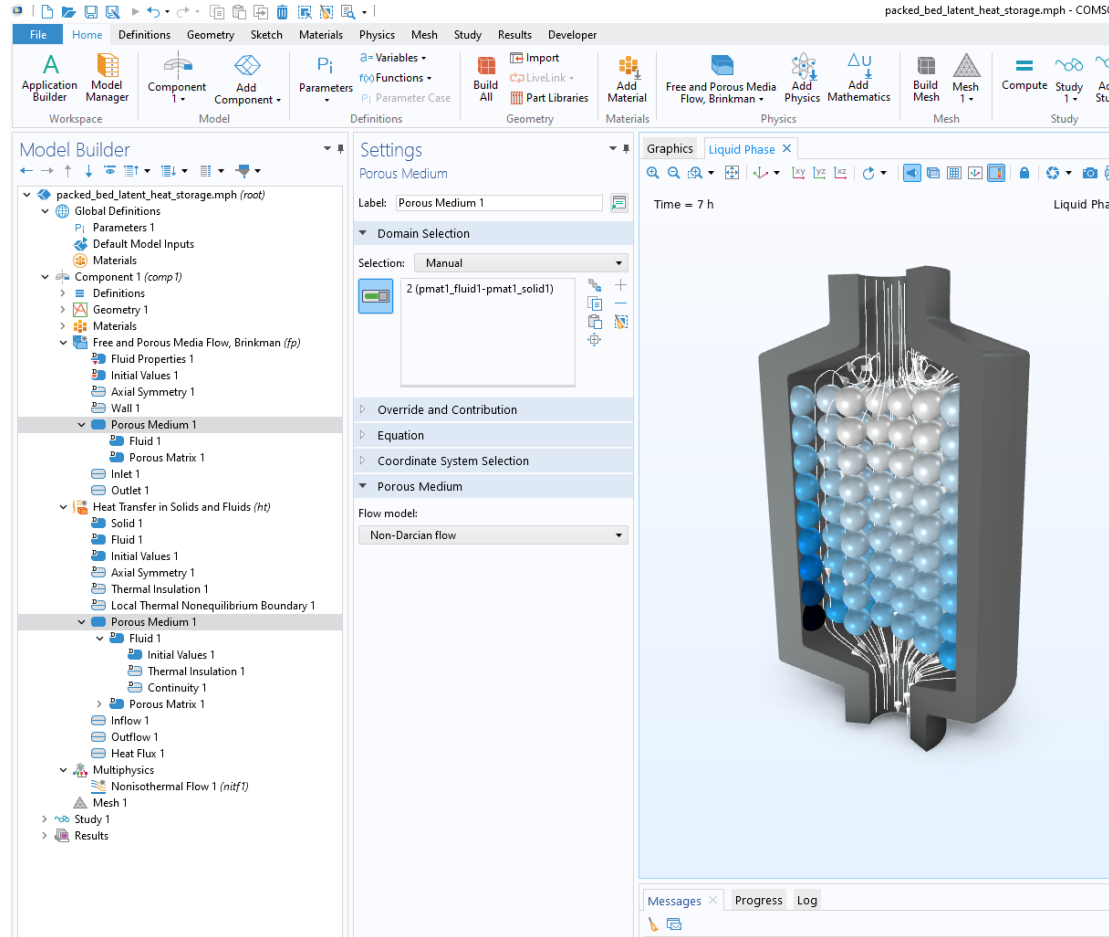
Modelling Porous Materials

Porous Medium

Feature available in various interfaces with settings specific for the physics that is solved.

Porous Material

Special Material to set up all the required properties for the different parts of the porous structure.



Porous Medium

- Feature that is available for various interfaces
- Depending on the interface, different settings apply

The screenshot shows the COMSOL Multiphysics model tree. Two instances of the 'Porous Medium' feature are highlighted with blue boxes:

- Top instance:** Located under the 'Free and Porous Media Flow, Brinkman (*fp*)' interface. Its sub-features are 'Fluid Properties 1', 'Initial Values 1', 'Axial Symmetry 1', 'Wall 1', 'Porous Medium 1' (highlighted), 'Fluid 1', and 'Porous Matrix 1'. Below it are 'Inlet 1' and 'Outlet 1'.
- Bottom instance:** Located under the 'Heat Transfer in Solids and Fluids (*ht*)' interface. Its sub-features are 'Solid 1', 'Fluid 1', 'Initial Values 1', 'Axial Symmetry 1', 'Thermal Insulation 1', 'Local Thermal Nonequilibrium Boundary 1', 'Porous Medium 1' (highlighted), 'Fluid 1' (with sub-features 'Initial Values 1', 'Thermal Insulation 1', and 'Continuity 1'), and 'Porous Matrix 1'. Below it are 'Inflow 1', 'Outflow 1', and 'Heat Flux 1'.

At the bottom of the tree, the 'Multiphysics' section contains 'Nonisothermal Flow 1 (*nitf1*)'.

Porous Medium

Flow model:
 Non-Darcian flow

Porous Medium

Porous medium type:
 Local thermal nonequilibrium

Interstitial convective heat transfer coefficient:
 Spherical pellets

Average diameter:
 d_{pe} m

Porous Medium

- Feature that is available for various interfaces
- Depending on the interface, different settings apply
- Subnodes hold material properties e.g. Fluid properties and Porous Matrix properties or additional effects can be added e.g. Thermal Dispersion

- Free and Porous Media Flow, Brinkman (*fp*)
 - Fluid Properties 1
 - Initial Values 1
 - Axial Symmetry 1
 - Wall 1
 - Porous Medium 1
 - Fluid 1
 - Porous Matrix 1
 - Inlet 1
 - Outlet 1
- Heat Transfer in Solids and Fluids (*ht*)
 - Solid 1
 - Fluid 1
 - Initial Values 1
 - Axial Symmetry 1
 - Thermal Insulation 1
 - Local Thermal Nonequilibrium Boundary 1
 - Porous Medium 1
 - Fluid 1
 - Initial Values 1
 - Thermal Insulation 1
 - Continuity 1
 - Porous Matrix 1
 - Inflow 1
 - Outflow 1
 - Heat Flux 1
- Multiphysics
 - Nonisothermal Flow 1 (*nif1*)

Porous Material

- Contains the material properties belonging to the porous medium itself but also includes the properties of each individual phase present within it.

The screenshot displays the COMSOL Multiphysics software interface. The top menu bar includes File, Home, Definitions, Geometry, Sketch, Materials, Physics, Mesh, Study, Results, and Developer. The main workspace shows the Model Builder tree on the left and the Settings panel on the right.

Model Builder Tree:

- packed_bed_latent_heat_storage.mph (root)
 - Global Definitions
 - Component 1 (comp1)
 - Definitions
 - Geometry 1
 - Materials
 - Water, liquid (mat1)
 - Paraffin, solid (mat2)
 - Paraffin, liquid (mat3)
 - Glass Wool (mat4)
 - Porous Material 1 (pmat1)
 - Fluid 1 (pmat1.fluid1)
 - Solid 1 (pmat1.solid1)
 - Immobile Fluid 1 (pmat1.imfluid1)
 - Basic (def)
 - Free and Porous Media Flow, Brinkman (fp)
 - Fluid Properties 1
 - Initial Values 1
 - Axial Symmetry 1
 - Wall 1
 - Porous Medium 1
 - Fluid 1
 - Porous Matrix 1
 - Inlet 1
 - Outlet 1
 - Heat Transfer in Solids and Fluids (ht)
 - Multiphysics
 - Mesh 1
 - Study 1
 - Results

Settings Panel (Porous Material):

2

Override

Porosity

$$\epsilon_p = 1 - \theta_{im} = 1 - (\theta_s + \theta_{imf})$$

— Volume fractions of immobile phases

Name	Material	Volume fraction
Solid 1 (pmat1.solid1)	Locally defined	1-por
Immobile Fluid 1 (pmat1.imfluid1)	Water, liquid (mat1)	0.01

Phase-Specific Properties

Property	Variable	Value	Unit	Phase
<input checked="" type="checkbox"/> Density	rho	rho(T)	kg/m ³	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Density	rho	rho(T)	kg/m ³	Immobile Fluid 1 (pmat1.imf...
<input checked="" type="checkbox"/> Density	rho_av	kg/m ³		Solid 1 (pmat1.solid1)
<input checked="" type="checkbox"/> Dynamic viscosity	mu	eta(T)	Pa·s	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Heat capacity at constant pressure	Cp	Cp(T)	J/(kg·K)	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Heat capacity at constant pressure	Cp	Cp(T)	J/(kg·K)	Immobile Fluid 1 (pmat1.imf...
<input checked="" type="checkbox"/> Thermal conductivity	k_iso ; ki...	k(T)	W/(m·K)	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Thermal conductivity	k_iso ; ki...	k(T)	W/(m·K)	Immobile Fluid 1 (pmat1.imf...

Homogenized Material

Material: Locally defined

Homogenized Properties

Property	Variable	Value	Unit	Property group
<input checked="" type="checkbox"/> Permeability	kappa_is...	1e-12	m ²	Basic
<input checked="" type="checkbox"/> Porosity	epsilon	0.48	1	Porous model

Porous Material

Which phases require definition is dictated by the physics involved, and the porous material detects what needs to be specified.

The screenshot displays the COMSOL Multiphysics interface. The Model Builder on the left shows a tree view for a model named 'packed_bed_latent_heat_storage.mph'. Under 'Materials', 'Porous Material 1 (pmat1)' is selected, showing its sub-nodes: 'Fluid 1 (pmat1.fluid1)', 'Solid 1 (pmat1.solid1)', 'Immobile Fluid 1 (pmat1.imfluid1)', and 'Basic (def)'. The 'Settings' window on the right shows the configuration for 'Porous Material 1'. The 'Porosity' section contains the equation $\epsilon = 1 - \theta_{im} = 1 - (\theta_s + \theta_{imf})$. Below it, a table lists the volume fractions of immobile phases:

Name	Material	Volume fraction
fluid 1 (pmat1.fluid1)	Locally defined	1-por
immobile fluid 1 (pmat1.imfluid1)	Water, liquid (mat1)	0.01

The 'Phase-Specific Properties' section contains a table of properties for the porous material:

Property	Variable	Value	Unit	Phase
<input checked="" type="checkbox"/> Density	rho	rho(T)	kg/m ³	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Density	rho	rho(T)	kg/m ³	Immobile Fluid 1 (pmat1.imf...)
<input checked="" type="checkbox"/> Density	rho_av	kg/m ³	kg/m ³	Solid 1 (pmat1.solid1)
<input checked="" type="checkbox"/> Dynamic viscosity	mu	eta(T)	Pa·s	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Heat capacity at constant pressure	Cp	Cp(T)	J/(kg·K)	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Heat capacity at constant pressure	Cp	Cp(T)	J/(kg·K)	Immobile Fluid 1 (pmat1.imf...)
<input checked="" type="checkbox"/> Thermal conductivity	k_iso ; ki...	k(T)	W/(m·K)	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Thermal conductivity	k_iso ; ki...	k(T)	W/(m·K)	Immobile Fluid 1 (pmat1.imf...)

The 'Homogenized Material' section shows 'Material: Locally defined'. The 'Homogenized Properties' section contains a table of properties for the homogenized material:

Property	Variable	Value	Unit	Property group
<input checked="" type="checkbox"/> Permeability	kappa_is...	1e-12	m ²	Basic
<input checked="" type="checkbox"/> Porosity	epsilon	0.48	1	Porous model

Porous Material

Porosity is calculated from specified volume fraction of all solid and immobile phases.

The screenshot displays the COMSOL Multiphysics software interface, specifically the 'Materials' tab for a 'Porous Material' definition. The 'Volume fractions of immobile phases' table is visible, showing the following data:

Name	Material	Volume fraction
Solid 1 (pmat1.solid1)	Locally defined	1-por
Immobile Fluid 1 (pmat1.imfluid1)	Water, liquid (mat1)	0.01

The 'Homogenized Properties' table is also visible, showing the following data:

Property	Variable	Value	Unit	Property group
Permeability	kappa_is...	1e-12	m ²	Basic
Porosity	epsilon	0.48	1	Porous model

Porous Material

Phase-Specific Properties such as for the solid, fluid, or immobile fluid phase are defined in the corresponding subnode of the Porous Material.

The screenshot shows the COMSOL Multiphysics software interface. The Model Builder on the left displays a tree view of the model structure. The Porous Material 1 (pmat1) node is selected, and its Phase-Specific Properties are displayed in a table at the bottom.

Model Builder Tree View:

- packed_bed_latent_heat_storage.mph (root)
 - Global Definitions
 - Component 1 (comp1)
 - Definitions
 - Geometry 1
 - Materials
 - Water, liquid (mat1)
 - Paraffin, solid (mat2)
 - Paraffin, liquid (mat3)
 - Glass Wool (mat4)
 - Porous Material 1 (pmat1)
 - Fluid 1 (pmat1.fluid1)
 - Solid 1 (pmat1.solid1)
 - Immobile Fluid 1 (pmat1.imfluid1)
 - Basic (def)
 - Free and Porous Media Flow, Brinkman (fp)
 - Fluid Properties 1
 - Initial Values 1
 - Axial Symmetry 1
 - Wall 1
 - Porous Medium 1
 - Fluid 1

Settings - Porous Material

2

Override

Porosity

$$\epsilon_p = 1 - \theta_{im} = 1 - (\theta_s + \theta_{imf})$$

— Volume fractions of immobile phases

Name	Material	Volume fraction
Solid 1 (pmat1.solid1)	Locally defined	1-por
Immobile Fluid 1 (pmat1.imfluid1)	Water, liquid (mat1)	0.01

Phase-Specific Properties

Property	Variable	Value	Unit	Phase
<input checked="" type="checkbox"/> Density	rho	rho(T)	kg/m ³	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Density	rho	rho(T)	kg/m ³	Immobile Fluid 1 (pmat1.imf...)
<input checked="" type="checkbox"/> Density	rho	rho_av	kg/m ³	Solid 1 (pmat1.solid1)
<input checked="" type="checkbox"/> Dynamic viscosity	mu	eta(T)	Pa·s	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Heat capacity at constant pressure	Cp	Cp(T)	J/(kg·K)	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Heat capacity at constant pressure	Cp	Cp(T)	J/(kg·K)	Immobile Fluid 1 (pmat1.imf...)
<input checked="" type="checkbox"/> Thermal conductivity	k_iso ; ki...	k(T)	W/(m·K)	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Thermal conductivity	k_iso ; ki...	k(T)	W/(m·K)	Immobile Fluid 1 (pmat1.imf...)

Phase-Specific Properties

Property	Variable	Value	Unit	Phase
<input checked="" type="checkbox"/> Density	rho	rho(T)	kg/m ³	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Density	rho	rho(T)	kg/m ³	Immobile Fluid 1 (pmat1.imf...)
<input checked="" type="checkbox"/> Density	rho	rho_av	kg/m ³	Solid 1 (pmat1.solid1)
<input checked="" type="checkbox"/> Dynamic viscosity	mu	eta(T)	Pa·s	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Heat capacity at constant pressure	Cp	Cp(T)	J/(kg·K)	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Heat capacity at constant pressure	Cp	Cp(T)	J/(kg·K)	Immobile Fluid 1 (pmat1.imf...)
<input checked="" type="checkbox"/> Thermal conductivity	k_iso ; ki...	k(T)	W/(m·K)	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Thermal conductivity	k_iso ; ki...	k(T)	W/(m·K)	Immobile Fluid 1 (pmat1.imf...)

Add Required Phase Nodes

Porous Material

Homogenized Properties refer to material properties that pertain not to individual phases but to the entire porous medium, such as permeability.

It is also applicable for interfaces without a specific porous medium features when the properties of the porous medium have already been homogenized, such as the Young's Modulus in structural mechanics.

The screenshot displays the COMSOL Multiphysics software interface. The **Model Builder** panel on the left shows a hierarchical tree structure for a model named "packed_bed_latent_heat_storage.mph". The tree includes sections for Global Definitions, Component 1 (comp 1), Materials, Free and Porous Media Flow, Brinkman (fp), Fluid Properties 1, Initial Values 1, Axial Symmetry 1, Wall 1, Porous Medium 1, Inlet 1, Outlet 1, Heat Transfer in Solids and Fluids (ht), Multiphysics, and Study 1. Under the Materials section, "Porous Material 1 (pmat1)" is selected, showing its sub-entities: Fluid 1 (pmat1.fluid1), Solid 1 (pmat1.solid1), Immobile Fluid 1 (pmat1.imfluid1), and Basic (def).

The **Settings** panel on the right is configured for "Porous Material 2". It shows the **Override** section with the **Porosity** property set to $\epsilon_p = 1 - \theta_{im} = 1 - (\theta_s + \theta_{imf})$. Below this, the **Volume fractions of immobile phases** are defined in a table:

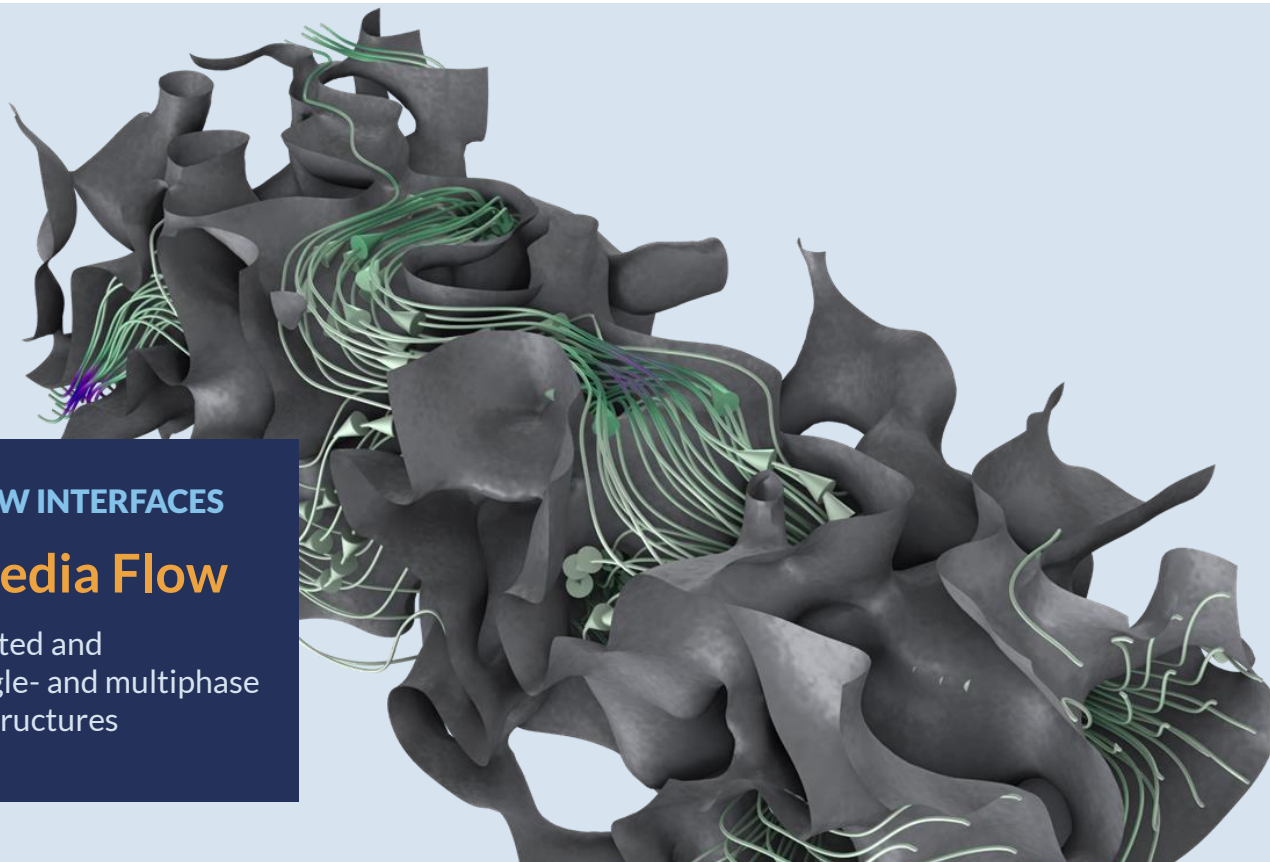
Name	Material	Volume fraction
Solid 1 (pmat1.solid1)	Locally defined	1-por
Immobile Fluid 1 (pmat1.imfluid1)	Water, liquid (mat1)	0.01

The **Phase-Specific Properties** section contains a table of properties for the porous material:

Property	Variable	Value	Unit	Phase
<input checked="" type="checkbox"/> Density	rho	rho(T)	kg/m ³	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Density	rho	rho(T)	kg/m ³	Immobile Fluid 1 (pmat1.imf...)
<input checked="" type="checkbox"/> Density	rho	rho_av	kg/m ³	Solid 1 (pmat1.solid1)
<input checked="" type="checkbox"/> Dynamic viscosity	mu	eta(T)	Pa·s	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Heat capacity at constant pressure	Cp	Cp(T)	J/(kg·K)	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Heat capacity at constant pressure	Cp	Cp(T)	J/(kg·K)	Immobile Fluid 1 (pmat1.imf...)
<input checked="" type="checkbox"/> Thermal conductivity	k_iso ; ki...	k(T)	W/(m·K)	Fluid 1 (pmat1.fluid1)
<input checked="" type="checkbox"/> Thermal conductivity	k_iso ; ki...	k(T)	W/(m·K)	Immobile Fluid 1 (pmat1.imf...)

At the bottom of the Settings panel, the **Homogenized Material** section is visible, showing the material set to "Locally defined". Below it, the **Homogenized Properties** section contains a table:

Property	Variable	Value	Unit	Property group
<input checked="" type="checkbox"/> Permeability	kappa_is...	1e-12	m ²	Basic
<input checked="" type="checkbox"/> Porosity	epsilon	0.48	1	Porous model

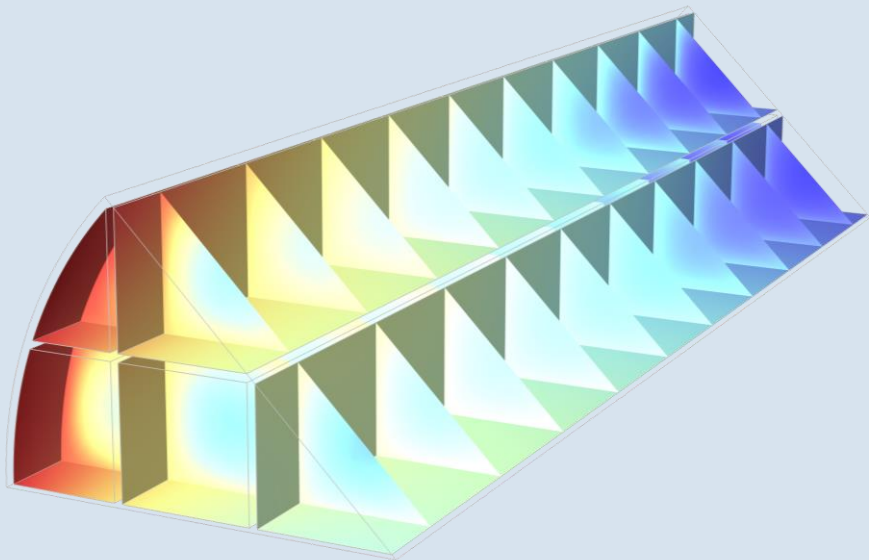


THE FLUID FLOW INTERFACES

Porous Media Flow

Modeling saturated and unsaturated single- and multiphase flow in porous structures

Darcy's Law



Background

Fundamental equation in hydrogeology to describe slow flow through porous media like soil or rocks, where velocity linearly depends on the pressure gradient

$$\nabla p = -\frac{\mu}{\kappa} \mathbf{u}$$

Permeability Models

Use anisotropic permeability, Kozeny-Carman, hydraulic conductivity, or even non-Darcian relationships

Applications

In petroleum and civil engineering and environmental science, and enabling efficient groundwater management, oil extraction, and pollution assessment

Storage Models

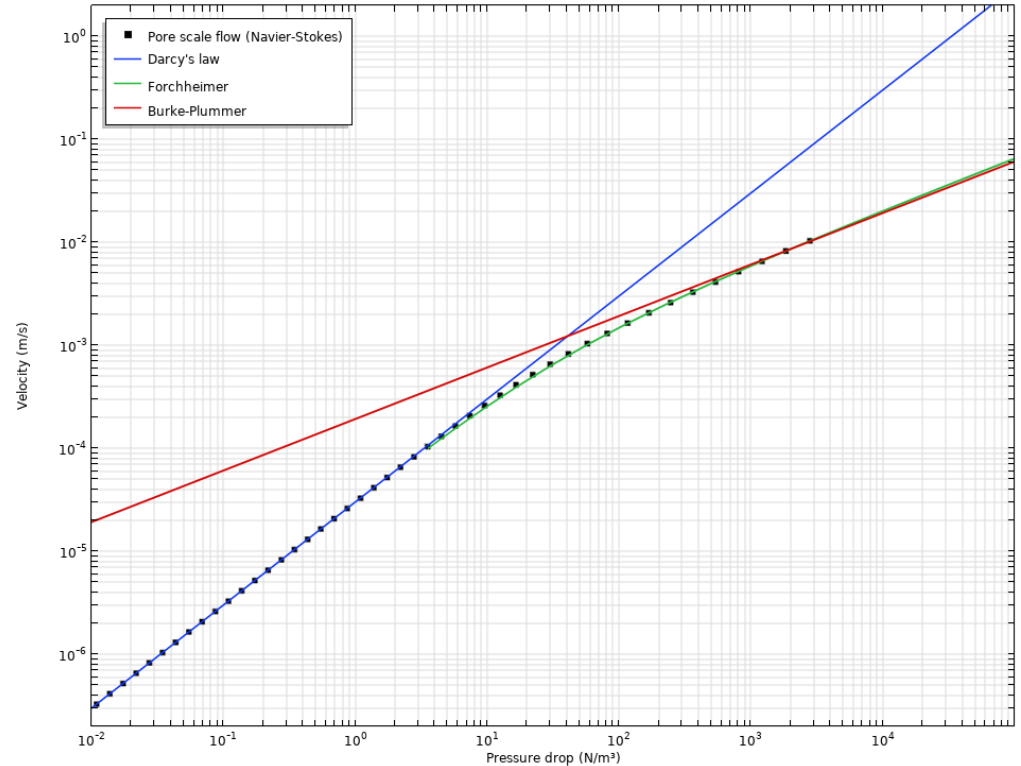
Include different storage models to account for water absorbed or released due to changes in hydraulic head

Non-Darcian Flow

- Non-Darcian flow options account for the nonlinear relationship between pressure drop and velocity:

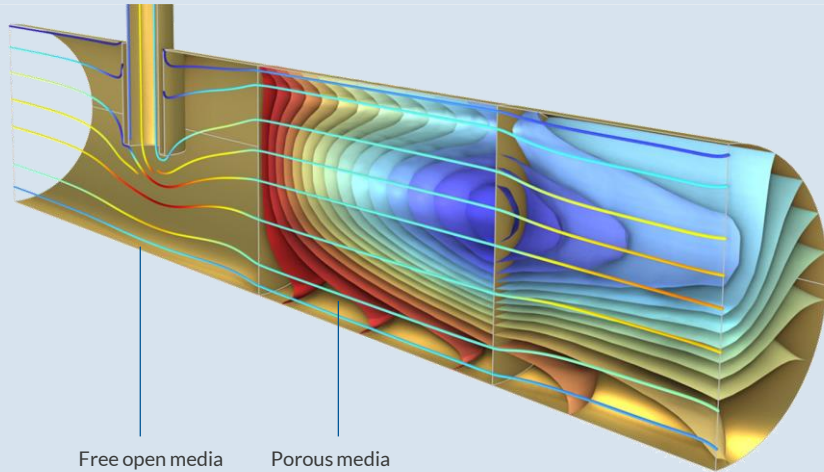
$$\nabla p = -\frac{\mu}{\kappa} \mathbf{u} - \beta \rho |\mathbf{u}| \mathbf{u}$$

- Forchheimer and Ergun ($Re < 1000$)
- Burke-Plummer ($Re > 1000$)
- Klinkenberg (gas slippage)



Comparison of the different permeability models with pore scale flow. Read more in the [COMSOL Blog post](#).

Brinkman Equations



Background

Modified Navier–Stokes equations (or extended Darcy’s law) for higher flow rates accounting for inertia and wall effects.

Applications

Wide range of applications for all kinds of porous materials like biophysics, filtration processes, and enhanced oil recovery

Extensions

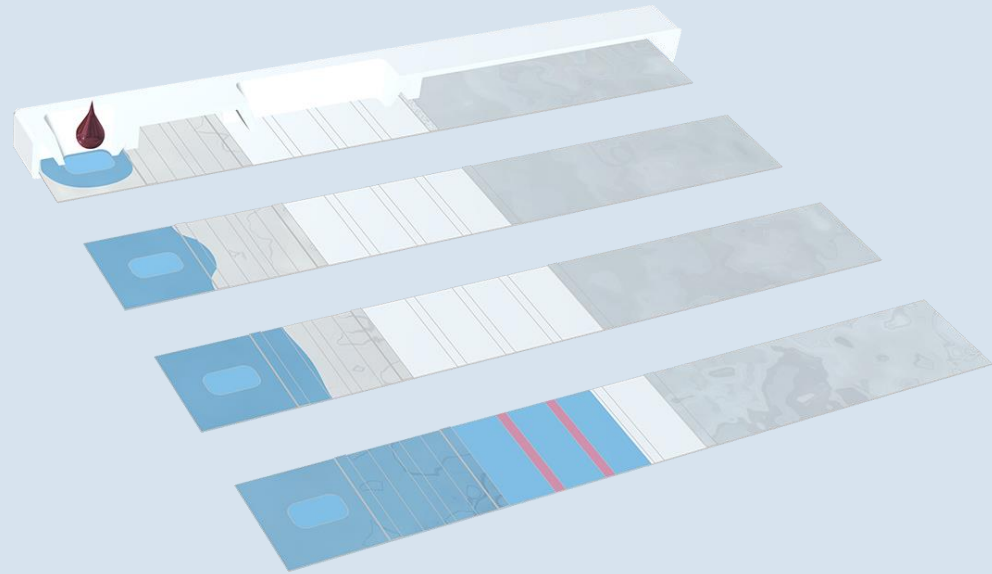
Porous slip wall treatment accounts for the slip condition walls, while the Forchheimer correction incorporates additional nonlinear resistance to the flow due to inertial effect

Turbulence

Keeps track of and conserves turbulence variables for flow through porous domains

Flow in Variable Saturated Porous Media

The Richards' Equation Interface



One Single Equation

That describes the movement of water through a partially saturated medium, where air pressure differences equilibrate quickly with atmospheric pressure, considering Darcy velocity only for the wetting phase

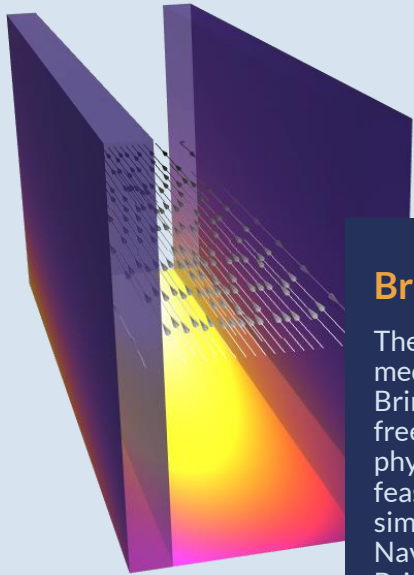
Retention Models

Interplay of moisture content, permeability, and water retention using Brooks–Corey, van Genuchten, or user-defined relationships

Storage Models

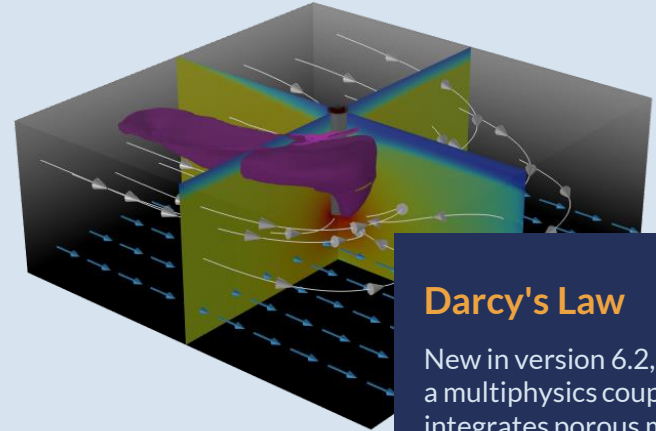
Account for storage of fluid using linearized or user-defined models or storage from liquid content

Free and Porous Media Flow



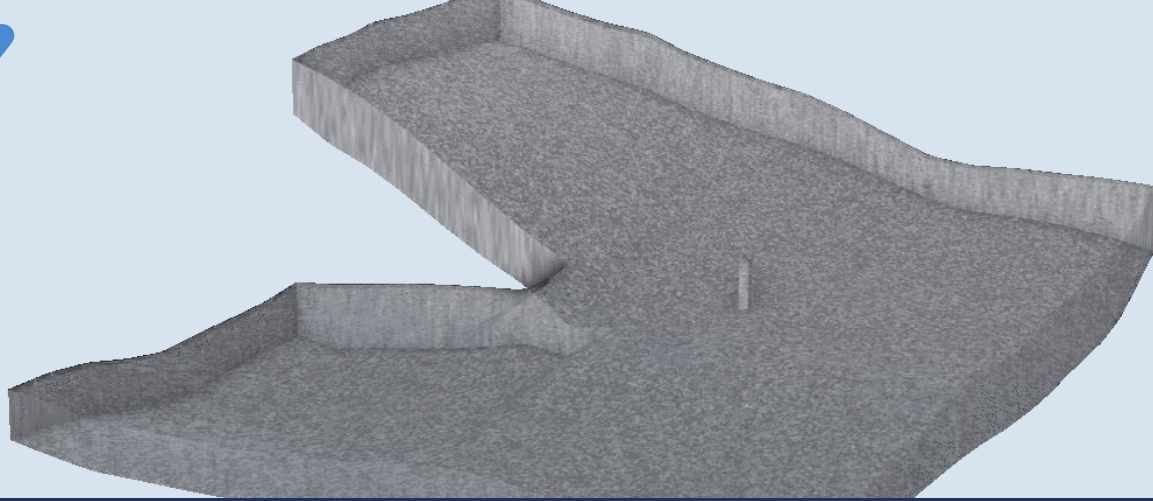
Brinkman Equations

The coupling of porous media flow governed by Brinkman equations with free flow is done in a single physics interface. This is feasible due to the striking similarity between the Navier–Stokes and Brinkman equations.



Darcy's Law

New in version 6.2, there is a multiphysics coupling that integrates porous media flow following Darcy's law and free flow. Boundary conditions are set at the interface between the free flow and porous media.



Multiphase Flow

Overview

Simultaneous movement of two or more distinct phases, such as gas, liquid, or solid particles, within a porous medium

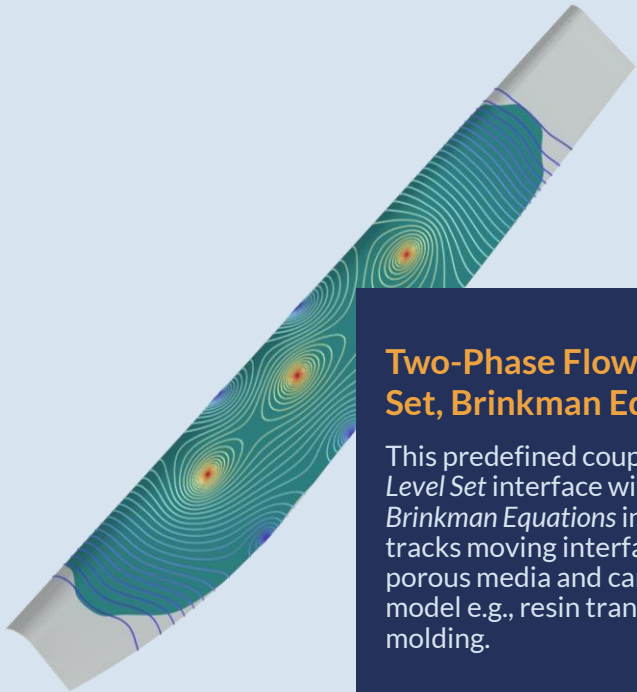
Applications

Enabling efficient resource extraction in the oil and gas industry, environmental remediation, drug delivery system optimization, and porous materials research

Challenges

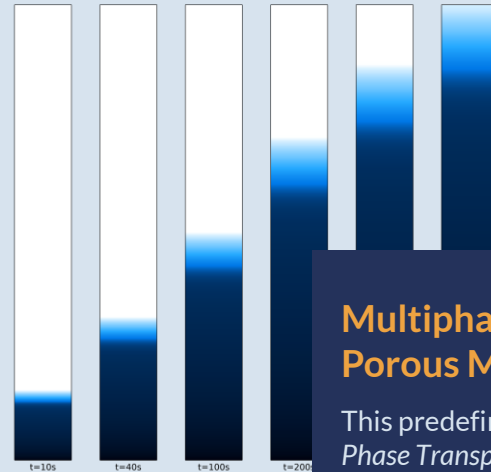
Complex phenomena due to interfacial tension, capillary pressure, and wettability, and phenomena like phase transitions and saturation changes

Multiphase Flow in Porous Media



Two-Phase Flow, Level Set, Brinkman Equations

This predefined coupling of a *Level Set* interface with a *Brinkman Equations* interface tracks moving interfaces in porous media and can be used to model e.g., resin transfer molding.

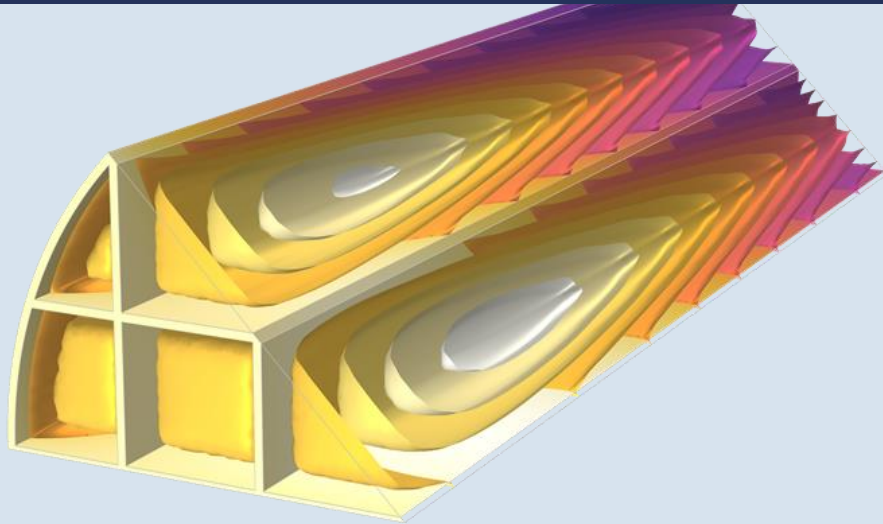


Multiphase Flow in Porous Media

This predefined coupling of the *Phase Transport in Porous Media* and *Darcy's Law* interfaces solves for the averaged volume fractions of the different phases.

Capillary diffusion is available.

Heat Transfer in Porous Media



Convection

Heat transfer in porous media, moist porous media, building materials, and fractures with velocity field from Darcy's law or Brinkman equations

Conduction

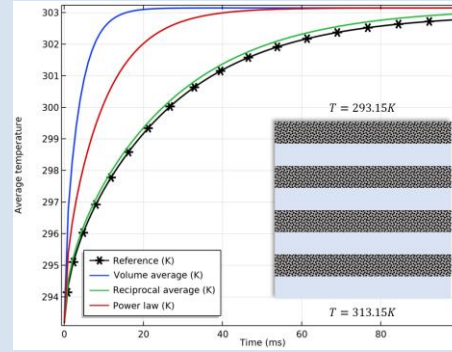
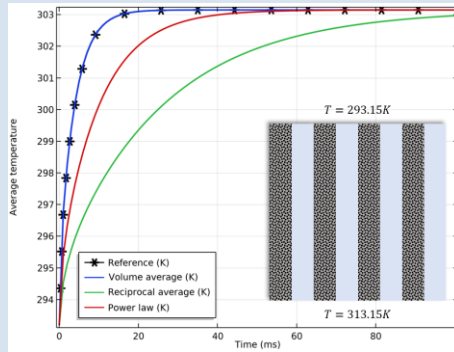
Effective values for material properties of different structures of porous materials, with up to five different immobile phases

Thermal Dispersion

Spreading of heat due to fluid movement within the porous structure, leading to a more uniform temperature distribution

Geothermal Heating

Add contributions from radiogenic heat production and geothermal gradients



Local Thermal Equilibrium

▼ Porous Medium

Porous medium type:

Local thermal equilibrium ▼

Effective thermal conductivity:

Fluid spherical inclusions ▼

Plane layers parallel to heat flow

Plane layers perpendicular to heat flow

Power law

Solid spherical inclusions

Fluid spherical inclusions

Wrapped screen

Sintered metal fibers

Equivalent thermal conductivity

- Temperature of the solid matrix and the fluid (and possible other phases) within the pores are the same at any given point and time
- Effective material properties are computed for the porous medium averaged over all phases
- Effective thermal conductivity depends on the structure of the porous medium

Local Thermal Nonequilibrium

- Solid and fluid temperature are not in local equilibrium
- Temperature differences can be substantial for fast nonisothermal flows, phase change, or on short time scales

packed_bed_latent_heat_storage.mph - COMSOL Multiphysics

File Home Definitions Geometry Sketch Materials Physics Mesh Study Results Developer

Application Builder Model Manager Component 1 Add Component Parameters Variables Functions Parameter Case Definitions Import LiveLink Build All Part Libraries Add Material Heat Transfer in Solids and Fluids Add Physics Add Mathematics Build Mesh Mesh 1 Compute Study 1 Add Study 3D Plot Group 9 Add Plot Group

Workspace Model Physics Mesh Study Results Developer

Model Builder

- packed_bed_latent_heat_storage.mph (root)
 - Global Definitions
 - Component 1 (comp 1) (comp 1)
 - Definitions
 - Geometry 1 (geom 1)
 - Materials
 - Free and Porous Media Flow, Brinkman (fp) (fp)
 - Heat Transfer in Solids and Fluids (ht) (ht)
 - Solid 1 (solid 1)
 - Fluid 1 (fluid 1)
 - Initial Values 1 (init 1)
 - Axial Symmetry 1 (axi 1)
 - Thermal Insulation 1 (ins 1)
 - Local Thermal Nonequilibrium Boundary 1 (ltneb 1)
 - Porous Medium 1 (porous 1)
 - Fluid 1 (fluid 1)
 - Initial Values 1 (init 1)
 - Thermal Insulation 1 (ins 1)
 - Continuity 1 (cont 1)
 - Porous Matrix 1 (pm 1)
 - Initial Values 1 (init 1)
 - Thermal Insulation 1 (ins 1)
 - Phase Change Material 1 (phc 1)
 - Inflow 1 (ifl 1)
 - Outflow 1 (ofl 1)
 - Heat Flux 1 (hfl 1)
 - Multiphysics
 - Mesh 1 (mesh 1)
 - Study 1 (std 1)
 - Results

Settings

Porous Medium

Label: Porous Medium 1

Domain Selection

Selection: Manual

2 (pmat1_fluid1-pmat1_solid1)

Override and Contribution

Equation

Coordinate System Selection

Global coordinate system

Porous Medium

Porous medium type: Local thermal nonequilibrium

Interstitial convective heat transfer coefficient: Spherical pellets

Average diameter: d_{pe} d_p m

Graphics Plot 1 X

Time=10.796 h Point: Porous matrix temperature=0.2

Local Thermal Nonequilibrium

- Fluid and Solid each have default boundary conditions (interaction with adjacent domains) and initial values.
- Additional subnodes are available for each phase.
- Local Thermal Nonequilibrium Boundary for two-temperature boundaries

packed_bed_latent_heat_storage.mph - COMSOL Multiphysics

File Home Definitions Geometry Sketch Materials Physics Mesh Study Results Developer

Application Builder Model Manager Component 1 Add Component Parameters Variables Functions Parameters Case Definitions Build All Import LiveLink Part Libraries Add Material Heat Transfer in Solids and Fluids Add Physics Add Mathematics Build Mesh Mesh 1 Compute Study 1 Add Study 3D Plot Group 9 Add Plot Group

Workspace Model Definitions Geometry Materials Physics Mesh Study

Model Builder

- packed_bed_latent_heat_storage.mph (root)
 - Global Definitions
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 - Materials
 - Free and Porous Media Flow, Brinkman (fp) (fp)
 - Heat Transfer in Solids and Fluids (ht) (ht)
 - Solid 1 (solid 1)
 - Fluid 1 (fluid 1)

Settings

Porous Medium

Label: Porous Medium 1

Domain Selection

Selection: Manual

2 (pmat1_fluid1-pmat1_solid1)

Override and Contribution

Equation

Coordinate System Selection

coordinate system:

Global coordinate system

Porous Medium

porous medium type:

Local thermal nonequilibrium

interstitial convective heat transfer coefficient:

Spherical pellets

Average diameter:

d_{pe} d_p m

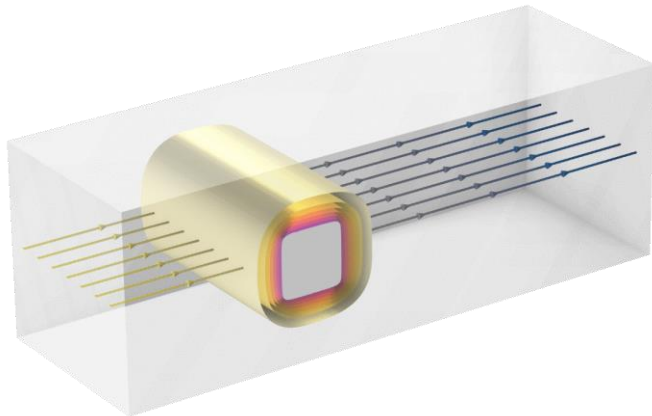
Graphics Plot 1 X

Time=10.796 h

Point: Porous matrix temperature=0.2

Phase Change in Porous Media

- Specify properties of each phase.
- Define the *Phase transition function*.
- Consider residual phases.



▼ Number of Phase Transitions

Number of phase transitions: 1

▶ Sketch

▼ Phase Change

Phase transition function: User defined

Latent heat from phase 1 to phase 2:
 $L_{1 \rightarrow 2}$ L J/kg

Phase transition between phase 1 and phase 2:
 $\alpha_{1 \rightarrow 2}$ f_phtr(T) 1

▼ Phase 1

Material, phase 1: Ice (mat3)

Thermal conductivity:
 k_1 From material

Density:
 ρ_1 From material

Heat capacity at constant pressure:
 $C_{p,1}$ From material

Ratio of specific heats:
 γ_1 Automatic

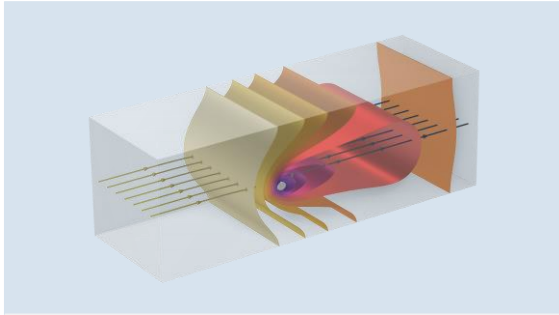
▶ Phase 2

Number of phase transitions

Define phase change function (linear, Heaviside, or user defined)

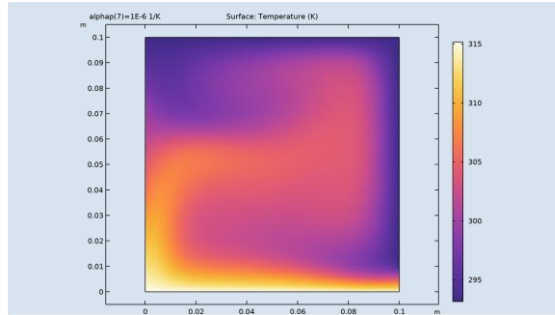
Set up material properties for each phase

Nonisothermal Flow



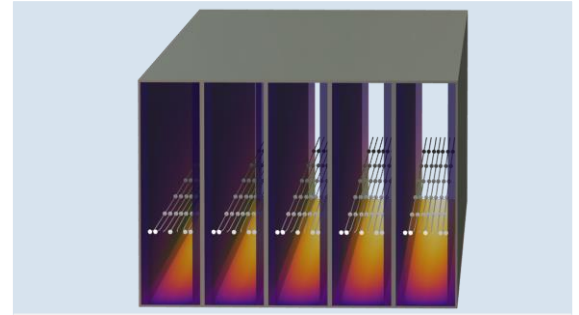
Material Properties

Understand the impact of temperature-dependent properties, such as viscosity, density, and thermal conductivity, on the fluid's behavior



Free Convection

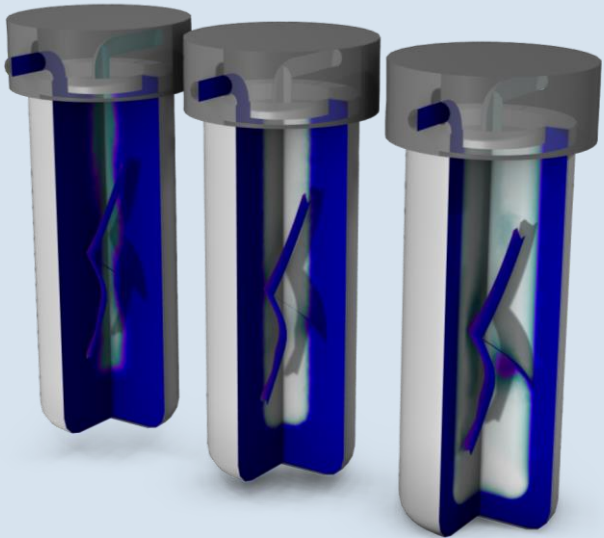
Buoyancy effects due to temperature gradients lead to density differences, driving natural convection. Use the Boussinesq approximation method to simplify the density variations in the buoyancy term



Viscous Dissipation

Conversion of mechanical energy into heat due to internal friction within the fluid, especially those involving high velocities or complex geometries

Solute Transport in Porous Media



Advection

Transport of diluted species in saturated and unsaturated porous media, with velocity field from Darcy's law, Richards' equation, or Brinkman equations

Adsorption

Adhering of solute to the surface of the porous structure using Langmuir, Freundlich, Toth, or Brunauer–Emmett–Teller (BET) isotherms

Volatilization

Volatile substances transition from liquid or solid phases to gas within porous materials, influencing, for example, the fate of pollutants

Diffusion

Effective diffusion accounting for the impact of the porous structure using the Millington–Quirk, Bruggeman, or Tortuosity formulations

Dispersion

Spreading of solutes as they move through the pore network due to mechanical mixing, diffusion, or the tortuosity of the flow paths

Transport of Diluted Species in Porous Media

- Effective diffusion:
 - Millington–Quirk
 - Bruggeman
 - Tortuosity
- Adsorption:
 - Langmuir
 - Freundlich
 - Toth
 - Brunauer–Emmett–Teller (BET)
- Dispersion
- Volatilization in partially saturated media

monolith_thermal_stress.mph - COMSOL Multiphysics

File Home Definitions Geometry Materials Physics Mesh Study Results Developer

Application Builder Model Manager 3D Model Add Component Parameters Variables Functions Import Build All LiveLink Part Libraries Add Material Transport of Diluted Species in Porous Media Add Physics Add Mathematics Build Mesh Mesh Compute Study Add Study

Workspace Model Definitions Geometry Materials Physics Mesh Study

Model Builder

Type filter text

- monolith_thermal_stress.mph
 - Global Definitions
 - Parameters 1
 - Default Model Inputs
 - Materials
 - Thermodynamics
 - Component 1
 - 3D Model
 - Definitions
 - Geometry 1(3D)
 - Materials
 - Chemistry 1
 - Transport of Diluted Species in Porous Media
 - Porous Medium 1
 - Fluid 1
 - Porous Matrix 1
 - No Flux 1
 - Initial Values 1
 - Reactions 1
 - Inflow 1
 - Outflow 1
 - Heat Transfer in Porous Media 1
 - Darcy's Law 1
 - Solid Mechanics
 - Multiphysics
 - Mesh 1
 - Study 1
 - Study 2
 - Study 3
 - Results

Settings

Fluid

Label: Fluid 1

- Domain Selection
- Equation
- Model Input
- Convection
- Diffusion
 - $D_{e,j} = D_{F,j}$
 - Source: Material
 - Fluid material: None
 - Fluid diffusion coefficient:
 - D_{F,CH_2O} User defined

pp1mat1.df4.D11	0	0	
0	0	0	m^2/s
0	0	0	
 - Diagonal
 - D_{F,CNH_3} User defined

pp1mat1.df1.D11	0	0	
0	0	0	m^2/s
0	0	0	
 - Diagonal
 - $D_{F,CNO}$ User defined

pp1mat1.df2.D11	0	0	
0	0	0	m^2/s
0	0	0	
 - Diagonal
 - D_{F,CO_2} User defined

pp1mat1.df3.D11	0	0	
0	0	0	m^2/s
0	0	0	
 - Diagonal

Graphics Conversion

0.96
0.9
0.83
0.76
0.7
0.63
0.57
0.5
0.43
0.37
0.3
0.23
0.17
0.1
0.03

z
y x

Log Messages Progress Table 2

Transport of Concentrated Species in Porous Media

- Diffusion models:
 - Maxwell–Stefan
 - Mixture-averaged
 - Fick's law
- Effective diffusion:
 - Millington–Quirk
 - Bruggeman
 - Tortuosity
- Knudsen diffusion
- Thermal diffusion

methane_steam_reformer_nirf.mph - COMSOL

File Home Definitions Geometry Sketch Materials Physics Mesh Study Results Developer

Application Builder Model Manager Component 2 Add Component Parameters Variables Functions Import Build All LiveLink Part Libraries Add Material Transport of Concentrated Species in Porous Media Add Physics Add Mathematics Build Mesh Mesh 1 Compute Study 2 Space dependent s

Workspace Model Definitions Geometry Materials Physics Mesh Study

Model Builder

Type filter text

- methane_steam_reformer_nirf.mph
 - Global Definitions
 - Parameters 1
 - Default Model Inputs
 - Materials
 - Thermodynamics
 - Component 1
 - Component 2
 - Definitions
 - Geometry 1(2Daxi)
 - Materials
 - Chemistry 1
 - Transport of Concentrated Species in Porous Media
 - Species Molar Masses
 - Porous Medium 1
 - Fluid 1
 - Porous Matrix 1
 - Initial Values 1
 - Axial Symmetry 1
 - No Flux 1
 - Reaction Sources 1
 - Inflow 1
 - Outflow 1
 - Free and Porous Media Flow 1
 - Fluid Properties 1
 - Initial Values 1
 - Axial Symmetry 1
 - Wall 1
 - Porous Medium 1
 - Inlet 1
 - Outlet 1
 - Heat Transfer in Porous Media 1
 - Multiphysics
 - Mesh 1
 - Study 1: Perfectly mixed model
 - Study 2: Space-dependent study
 - Results

Settings

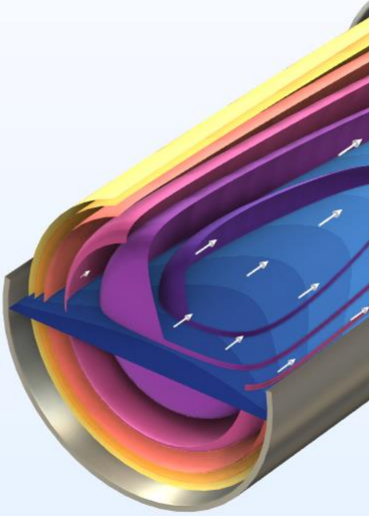
Fluid

Label: Fluid 1

- Domain Selection
- Equation
- Model Input
- Density
- Convection
 - Velocity field:
 - u Velocity field (nirf)
- Diffusion
 - Binary diffusion input type:
 - Table
 - Maxwell-Stefan diffusivities

| Species | Species | Diffusivity | Diffusion coefficient (m ² /s) |
|---------|---------|----------------|---|
| wCH4 | wCO | Maxwell-Stefan | comp2.chem.D_CH4_CO |
| wCH4 | wCO2 | Maxwell-Stefan | comp2.chem.D_CH4_CO2 |
| wCH4 | wH2 | Maxwell-Stefan | comp2.chem.D_CH4_H2 |
| wCH4 | wH2O | Maxwell-Stefan | comp2.chem.D_CH4_H2O |
 - Thermal diffusion coefficient
 - D_{wCH4}^T 0 kg/(m-s)
 - D_{wCO}^T 0 kg/(m-s)
 - D_{wCO2}^T 0 kg/(m-s)
 - D_{wH2}^T 0 kg/(m-s)
 - D_{wH2O}^T 0 kg/(m-s)
 - Effective diffusivity model:
 - Millington and Quirk model
 - Pore-Wall Interaction

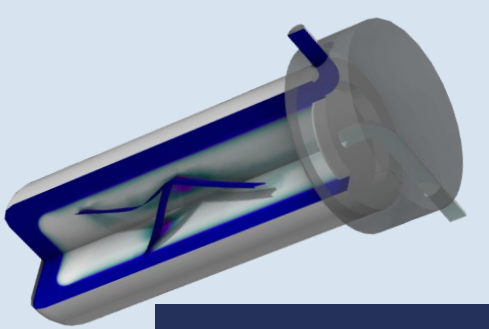
Graphics Temperature



Log Messages Progress Evaluation 3D

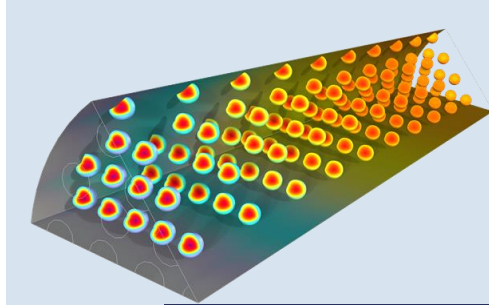
$$f_e = \frac{\epsilon_D}{\tau_F}, \tau_{F,j} = \epsilon_p^{-2/3}$$

Porous Medium Types



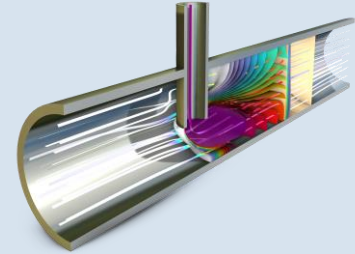
Porous Medium

Transport and reactions in pore space of solid matrix. Also transport along fractures in porous media and in unsaturated porous media.



Packed Bed

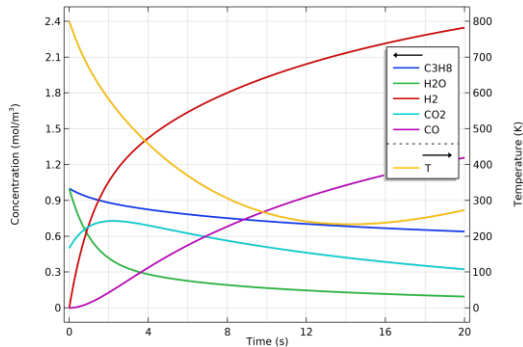
Porous catalytic particles in a fixed bed reactor. Models transport inside particles as well as in the bed macropores.



Porous Catalyst

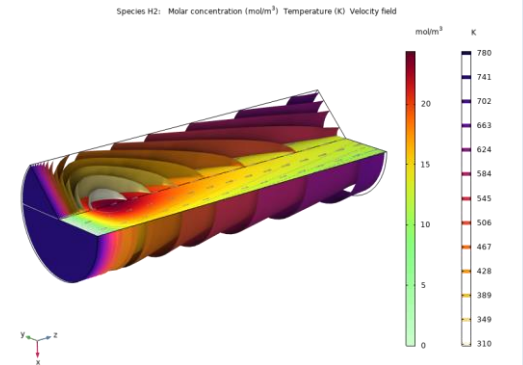
Extended support for heterogeneous reactions, adsorption, and desorption in porous media structures.

Chemical Reaction Engineering Module: Modeling Strategy



| Species | | | |
|-----------------|-----------|------------------|----------|
| Name | CAS | Chemical formula | Database |
| carbon dioxide | 124-38-9 | CO2 | COMSOL |
| carbon monoxide | 630-08-0 | CO | COMSOL |
| hydrogen | 1333-74-0 | H2 | COMSOL |
| propane | 74-98-6 | C3H8 | COMSOL |
| water | 7732-18-5 | H2O | COMSOL |

| Phases | |
|--------|-------|
| Name | State |
| Gas | Vapor |



Perfectly Mixed System

- Type in the chemical equations
- Kinetics and material balances automatically formulated

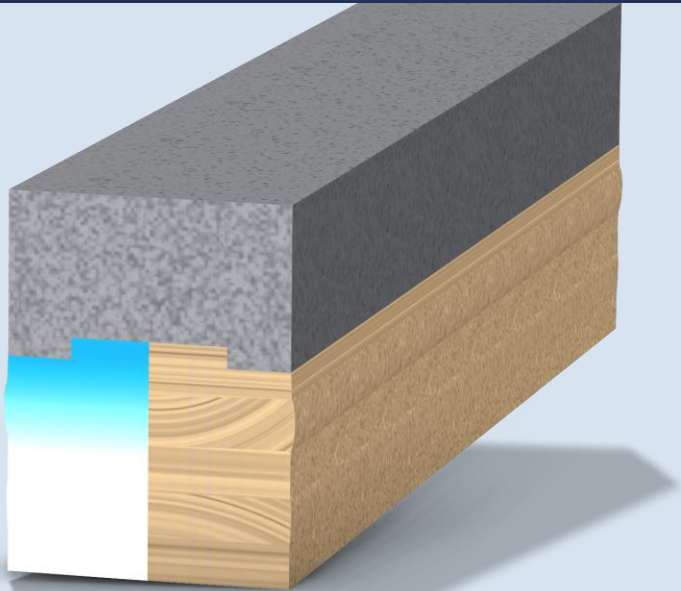
Thermodynamic Properties

- Add a thermodynamic system
- Add compounds
- Match species

Generate Space-Dependent Model

- Select space dimension
- Select transport mechanism for chemical species, fluid flow, and heat transfer

Moisture Transport in Porous Media



Transport Mechanisms

Moisture moves through convection and diffusion, facilitated by the presence of both vapor and liquid states within the pores.

Liquid Water

Held by adsorption (vapor molecules adhering to pore walls) and capillarity (pressure difference between liquid and gas phases).

Moisture

Hygroscopic and capillary regions based on the dominance of adsorption or capillarity, respectively, influenced by factors like relative humidity and pore characteristics.

Characterization

Moisture is characterized through sorption curves (for hygroscopic region) and retention curves (for capillary region), employing models like van Genuchten and Brooks & Corey.

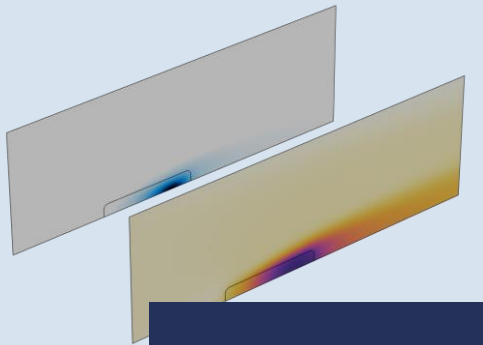
State Variables

Relative humidity and capillary pressure are termed state variables, describing water's thermodynamic state in equilibrium between phases, governed by Kelvin's law.

Porous Matrix

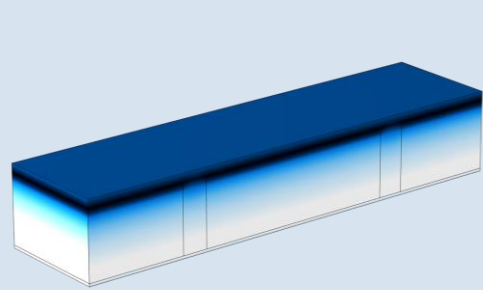
Liquid saturation and moisture content are dependent on the structure, varying with factors such as porosity, pore size distribution, and material composition.

Moisture Transport in Porous Media



Hygroscopic Porous Medium

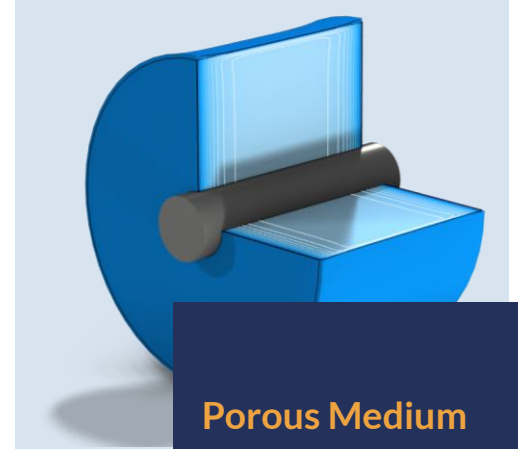
Moisture transport in a porous medium filled with liquid water and moist air by vapor diffusion and convection in moist air, and convection and capillary flow in the liquid phase.



Building Material

Moisture transfer through vapor diffusion and capillary moisture flows.

Specific equations for building materials under typical external conditions.

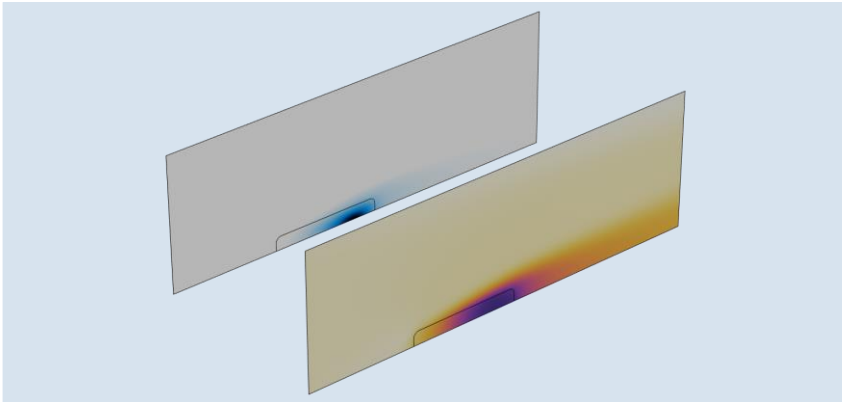


Porous Medium

Moisture transport in conjunction with deforming materials.

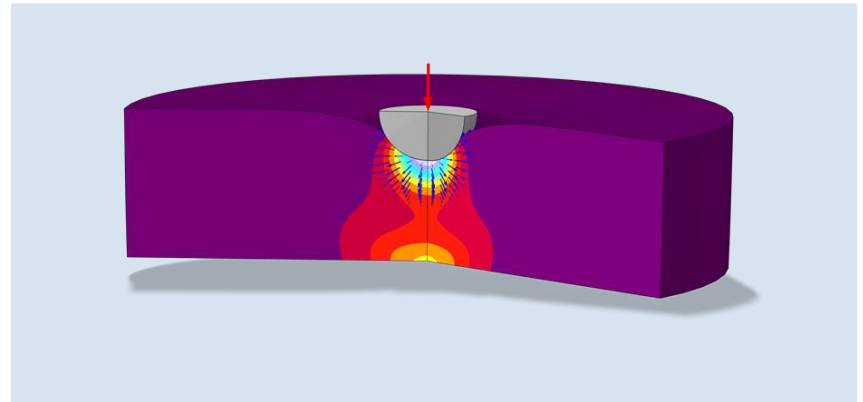
Accurate mass and energy conservation with large deformations.

Multiphysics Capabilities



Heat and Moisture

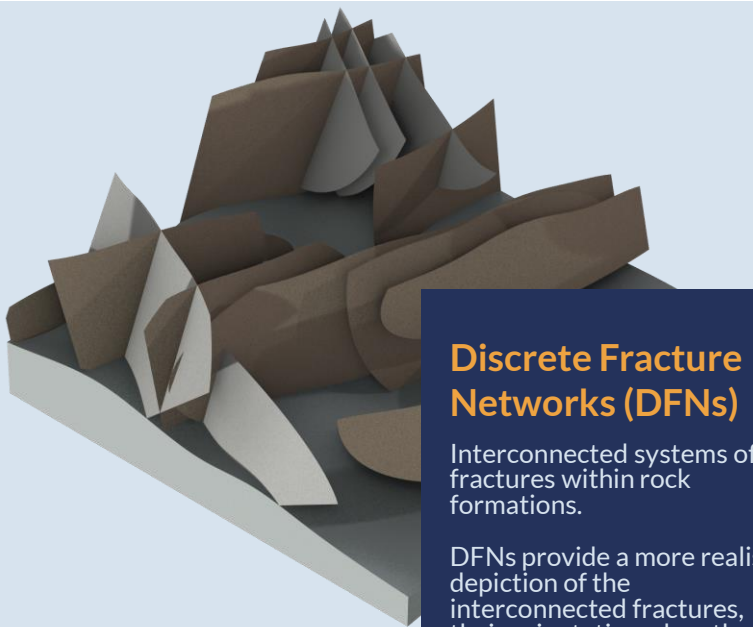
- Take into account heat and moisture storage, latent heat, and heat and moisture transport
- Relative humidity depends on temperature and pressure



Poroelasticity

- Compaction and swelling of saturated and unsaturated porous materials:
 - Biot: General framework, applicable to a wide range of porous materials.
 - Biphase: Suitable for modeling the coupling between fluid flow and large deformations in hydrogels and soft biological tissues

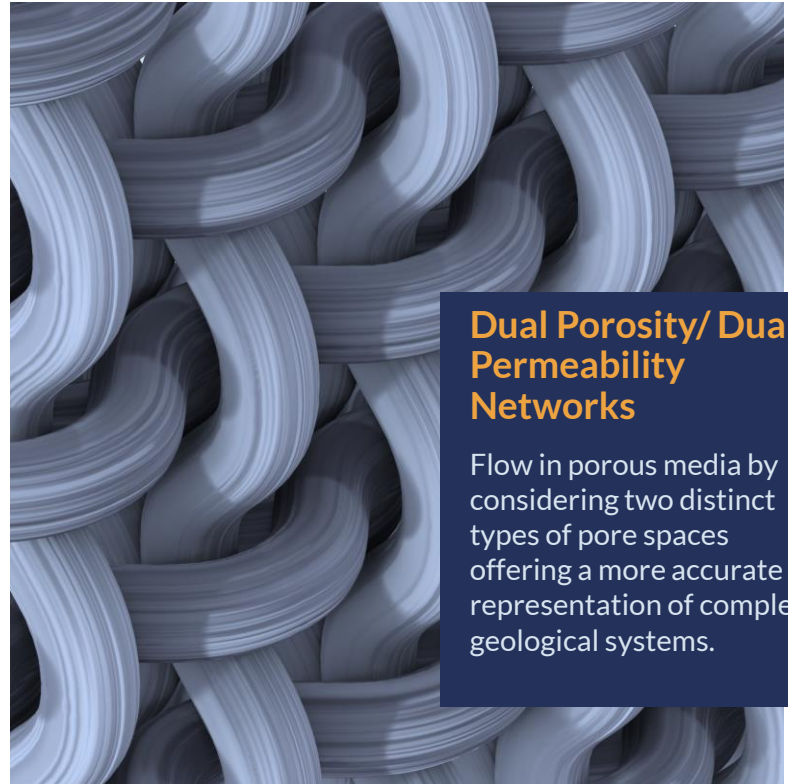
Complex Porous Materials



Discrete Fracture Networks (DFNs)

Interconnected systems of fractures within rock formations.

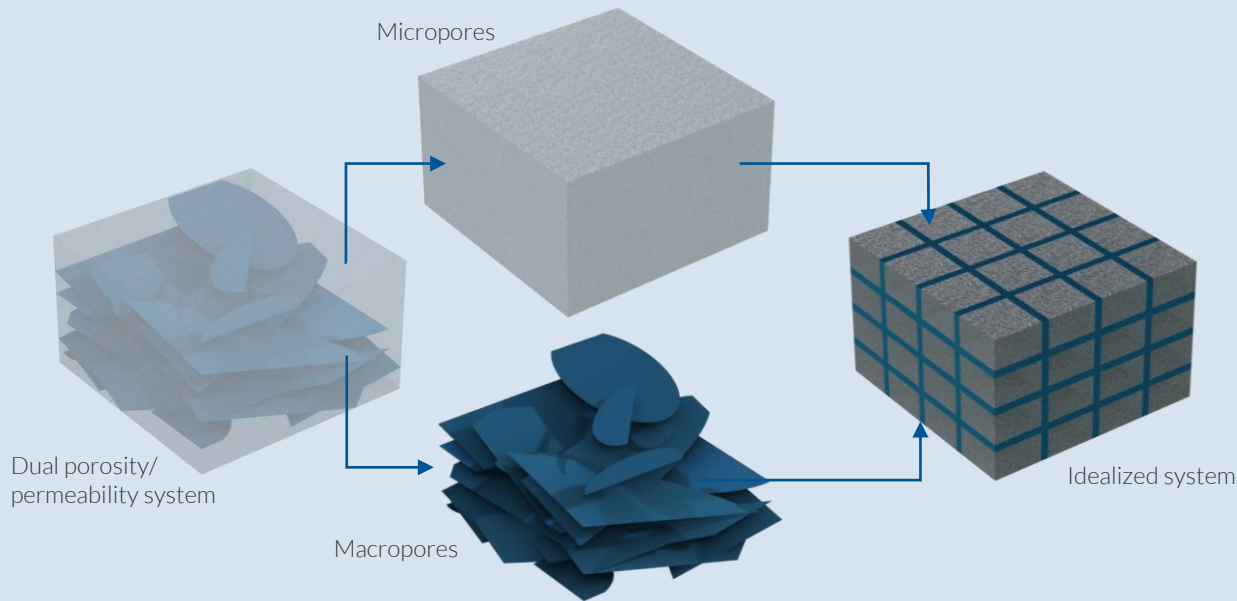
DFNs provide a more realistic depiction of the interconnected fractures, their orientations, lengths, and aperture distributions.



Dual Porosity/ Dual Permeability Networks

Flow in porous media by considering two distinct types of pore spaces offering a more accurate representation of complex geological systems.

Dual Porosity and Dual Permeability



Macropores

- Highly conductive regions within a rock or geological formation that significantly impact fluid flow and transport
- Usually occupy only a small fraction of the whole system

Micropores

- Regions with low permeability occupying a large volume fraction of the whole system
- Contribute significantly to storage capacity within a geological formation

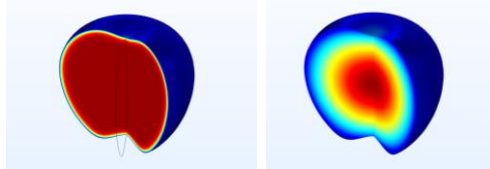
INNOVATION AT Empa

Forecasting Produce Shelf Life

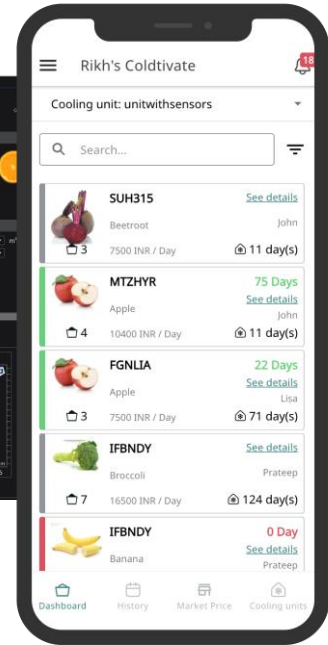
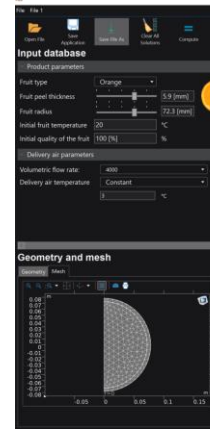
Each year, approximately one-third of the food produced for human consumption worldwide is lost or wasted. To optimize the use of refrigerated food storage in developing countries, farmers and traders need to be able to predict the shelf life of fresh fruits and vegetables.

Minimizing post-harvest losses with limited refrigerated space available requires insight into how ambient temperatures directly influence the shelf life of fresh produce.

The EMPA team compiled a simulation app from their multiphysics models to provide data-driven forecasts on the freshness of produce in a cold room. Results from the simulation app are fed into a smartphone app.



The Coldtivate mobile app informs farmers and cold storage operators of the cooling and decay process of different types of produce in real time. The values shown in the app are recalculated every 6 hours based on the latest cold room temperature data.



In August 2022, the simulation-powered app was released to 17 cold rooms, serving more than 300 farmers, who are reporting a 20% increase in their incomes and reduction of their post-harvest food losses.

Empa and its partners are now working to expand Coldtivate's impact.



SIMULATION APP HETT²²

A leading global cement supplier provides its customers with a standalone simulation app that predicts curing times for concrete casting at construction sites. Since launch, it has been downloaded 1500 times!

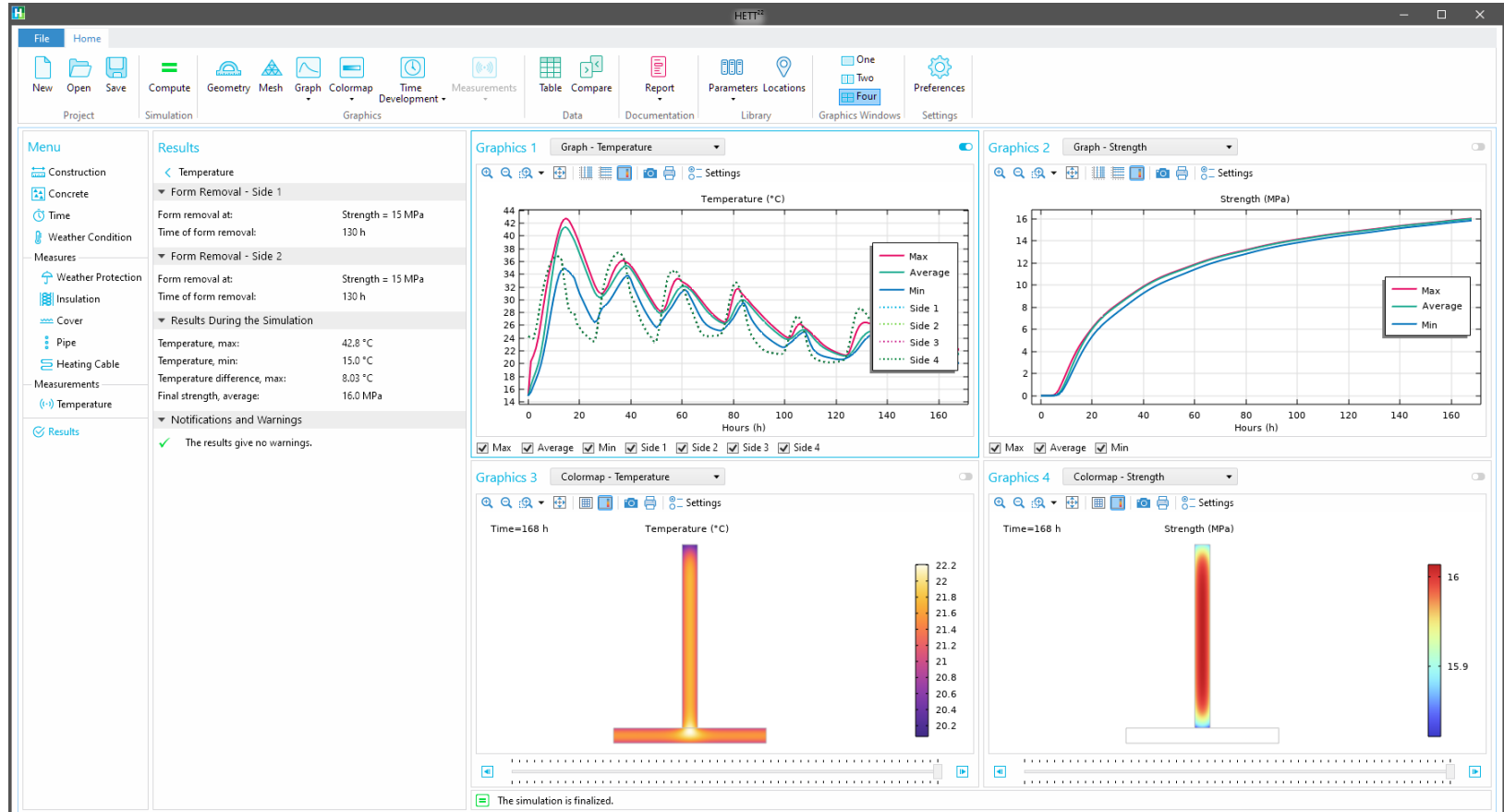
SIMULATION APP HETT²²

- The app user chooses the concrete and cement mixture based on weather and construction structure
- Uses data from weather stations to determine the conditions for the curing process in real time
- The output from the simulation app:
 - Predicts temperature, degree of curing, and structural properties
 - Warns if the structural integrity of the structure is at risk

Developed by Deflexional AB
(COMSOL Certified Consultant)

deflexional 





Concluding Remarks

Extensive Modelling Features

COMSOL Multiphysics® offers user-friendly tools for modeling porous media flow, heat and solute transport, and additional phenomena, such as poroelasticity.

Ready-Made and User-Defined Multiphysics

Multiphysics interfaces are available for nonisothermal porous media flow, multiphase transport, reacting flow, and poroelasticity. It is also straightforward to define arbitrary couplings.

