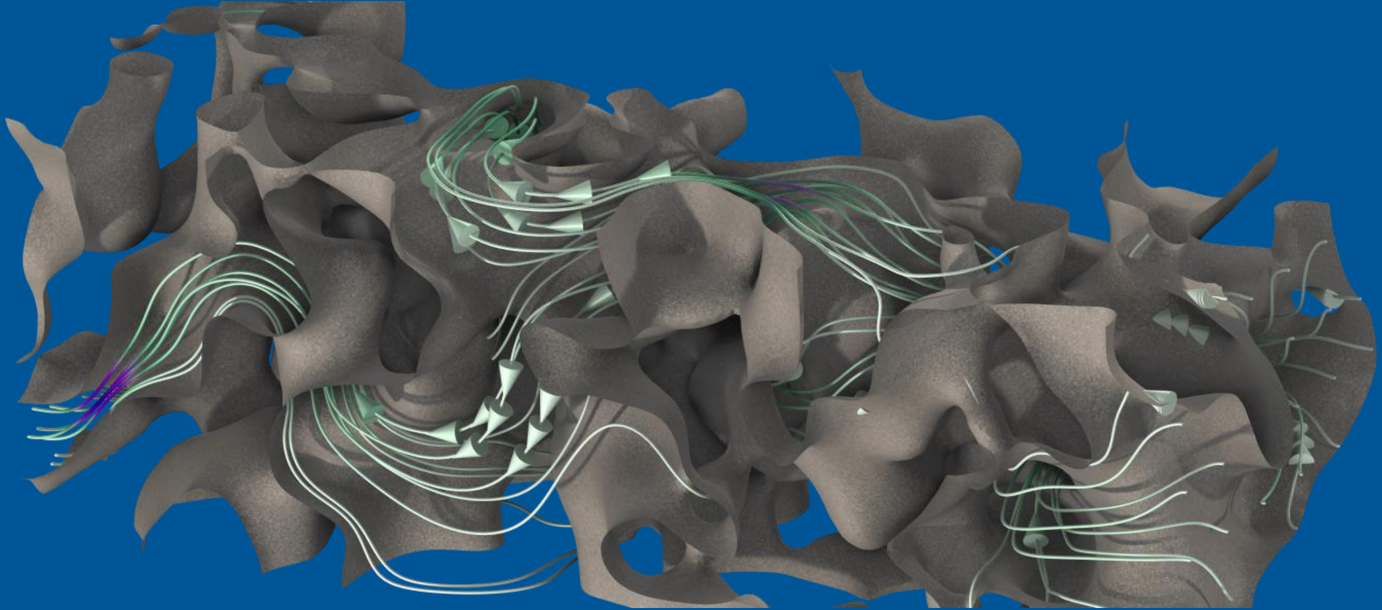
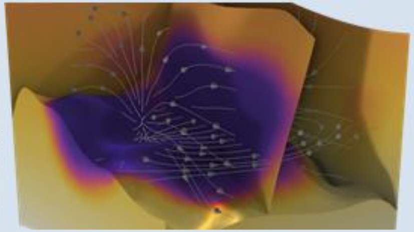


Heat and Moisture Transport in Porous Media

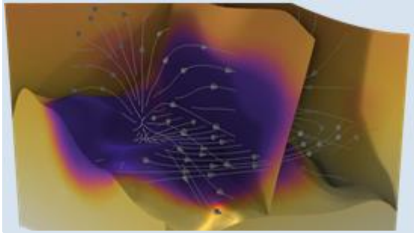
Nancy Bannach
COMSOL

Diversity of Porous Media

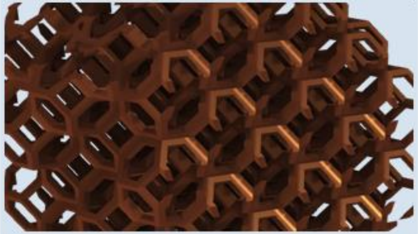


Geothermal Reservoirs

Diversity of Porous Media

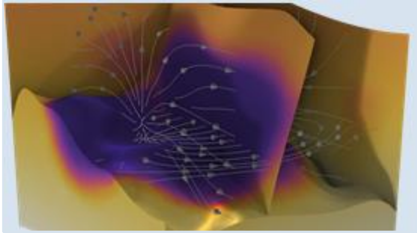


Geothermal Reservoirs

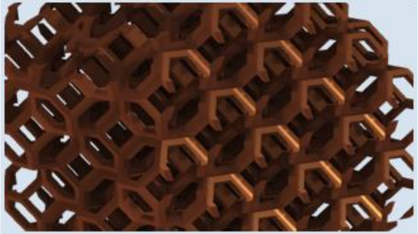


Material Science

Diversity of Porous Media



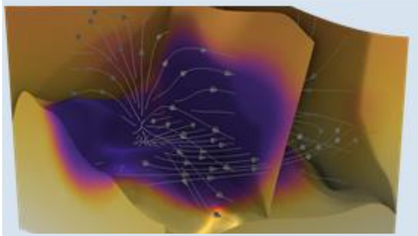
Geothermal Reservoirs



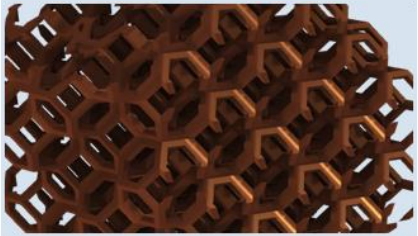
Material Science

Healthcare Applications

Diversity of Porous Media

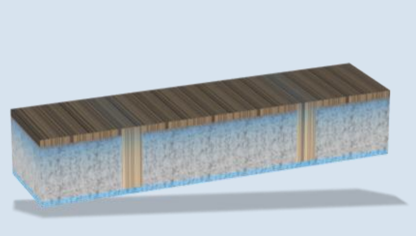


Geothermal Reservoirs



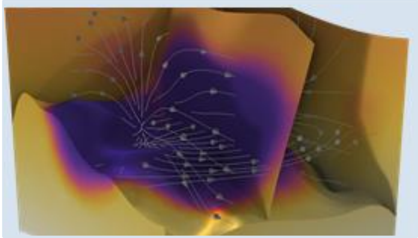
Material Science

Healthcare Applications

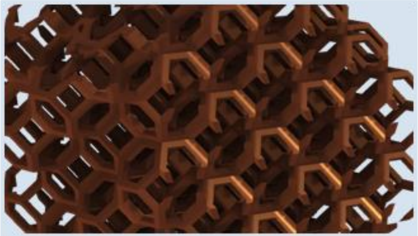


Building & Construction

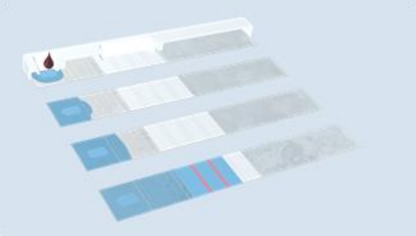
Diversity of Porous Media



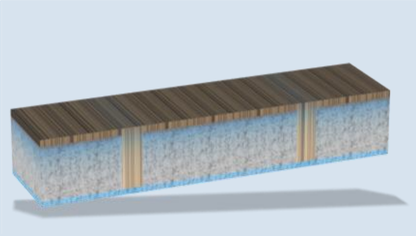
Geothermal Reservoirs



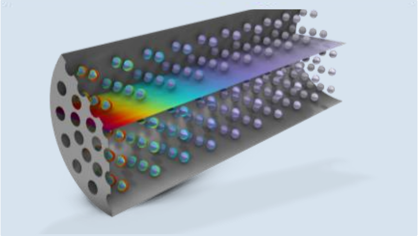
Material Science



Healthcare Applications

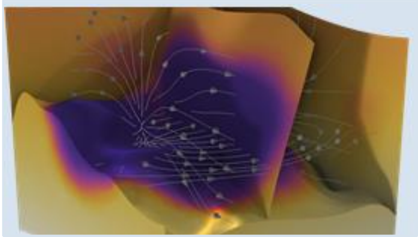


Building & Construction

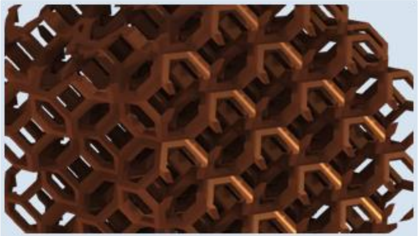


Packed Bed Reactor

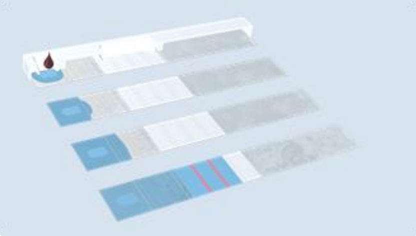
Diversity of Porous Media



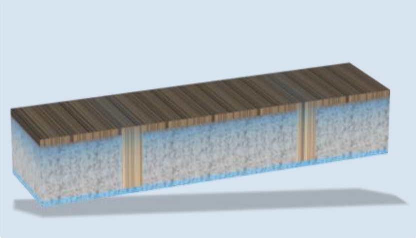
Geothermal Reservoirs



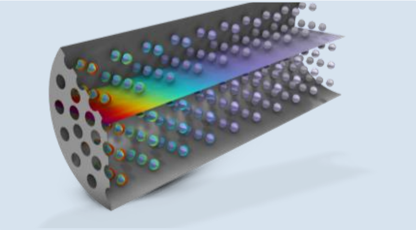
Material Science



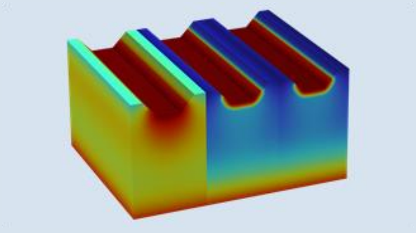
Healthcare Applications



Building & Construction

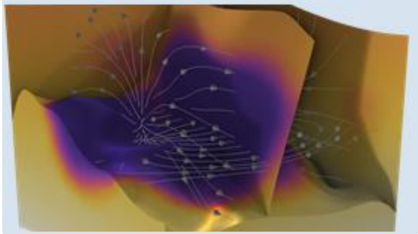


Packed Bed Reactor

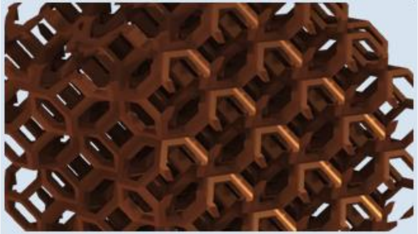


Agriculture Applications

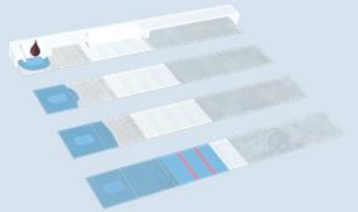
Diversity of Porous Media



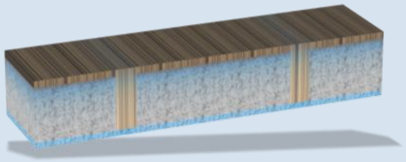
Geothermal Reservoirs



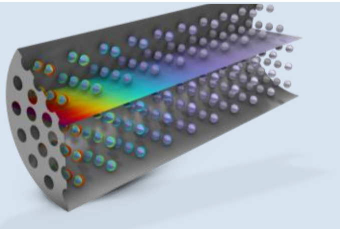
Material Science



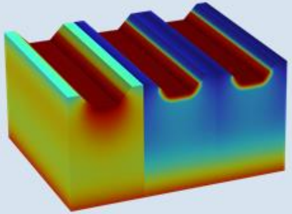
Healthcare Applications



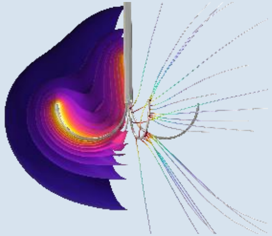
Building & Construction



Packed Bed Reactor

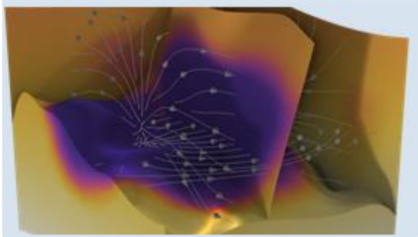


Agriculture Applications

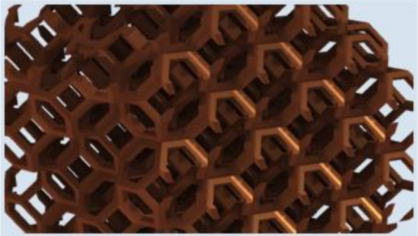


Biological Tissue

Diversity of Porous Media

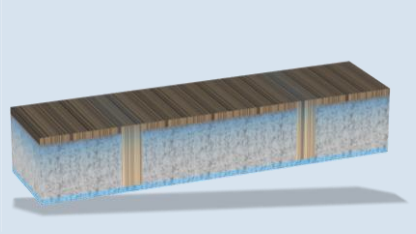


Geothermal Reservoirs

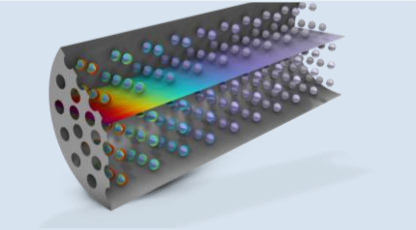


Material Science

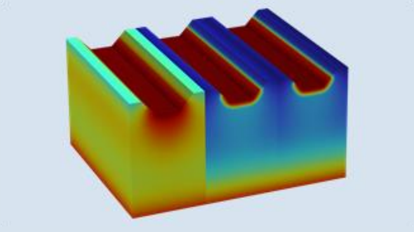
Healthcare Applications



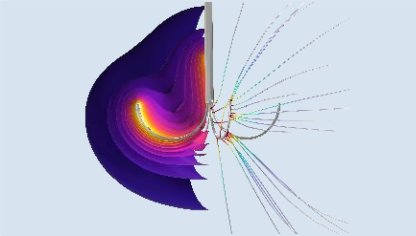
Building & Construction



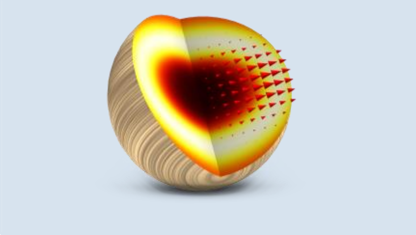
Packed Bed Reactor



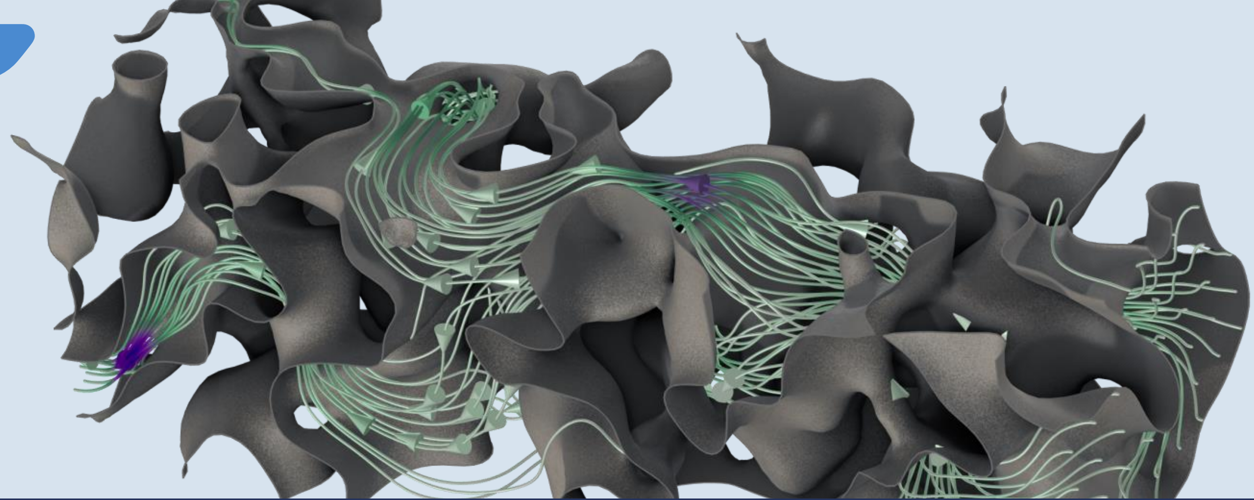
Agriculture Applications



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

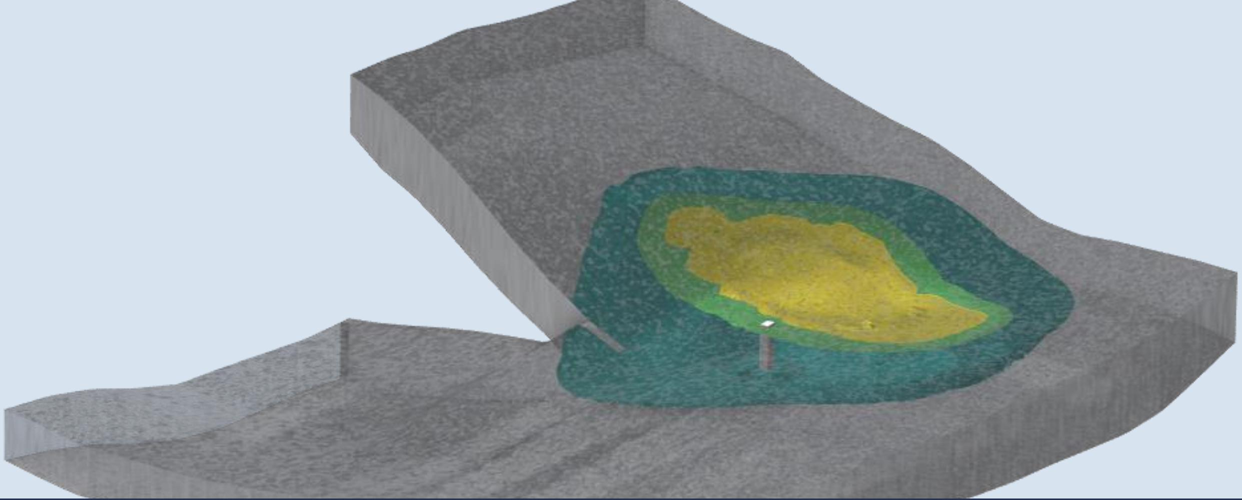
Predicting permeability, understanding multiphase flow, and simulating fluid behavior in biological tissues

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™
Host and administrate your simulation apps. Run them through a web interface.

ADD-ON PRODUCTS

ELECTROMAGNETICS

- AC/DC Module
- RF Module
- Wave Optics Module
- Ray Optics Module
- Plasma Module
- Semiconductor Module

FLUID & HEAT

- 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

INTERFACING

- LiveLink™ *for* MATLAB®
- LiveLink™ *for* Simulink®
- LiveLink™ *for* Excel®
- CAD Import Module
- Design Module
- ECAD Import Module
- LiveLink™ *for* SOLIDWORKS®
- LiveLink™ *for* Inventor®
- LiveLink™ *for* AutoCAD®
- LiveLink™ *for* Revit®
- LiveLink™ *for* PTC Creo Parametric™
- LiveLink™ *for* Solid Edge®
- File Import *for* CATIA® V5

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™

Host and administrate your simulation apps. Run them through a web interface.

ADD-ON PRODUCTS

ELECTROMAGNETICS

- AC/DC Module
- RF Module
- Wave Optics Module
- Ray Optics Module
- Plasma Module
- Semiconductor Module

FLUID & HEAT

- CFD Module
  - Mixer Module
- Polymer Flow Module
- Microfluidics Module
- Porous Media Flow Module
- Subsurface 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

INTERFACING

- LiveLink™ *for* MATLAB®
- LiveLink™ *for* Simulink®
- LiveLink™ *for* Excel®
- CAD Import Module
- Design Module
- ECAD Import Module
- LiveLink™ *for* SOLIDWORKS®
- LiveLink™ *for* Inventor®
- LiveLink™ *for* AutoCAD®
- LiveLink™ *for* Revit®
- LiveLink™ *for* PTC Creo Parametric™
- LiveLink™ *for* Solid Edge®
- File Import *for* CATIA® V5

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™

Host and administrate your simulation apps. Run them through a web interface.

ADD-ON PRODUCTS

ELECTROMAGNETICS

- AC/DC Module
- RF Module
- Wave Optics Module
- Ray Optics Module
- Plasma Module
- Semiconductor Module

FLUID & HEAT

- 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

INTERFACING

- LiveLink™ *for* MATLAB®
- LiveLink™ *for* Simulink®
- LiveLink™ *for* Excel®
- CAD Import Module
- Design Module
- ECAD Import Module
- LiveLink™ *for* SOLIDWORKS®
- LiveLink™ *for* Inventor®
- LiveLink™ *for* AutoCAD®
- LiveLink™ *for* Revit®
- LiveLink™ *for* PTC Creo Parametric™
- LiveLink™ *for* Solid Edge®
- File Import *for* CATIA® V5

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™

Host and administrate your simulation apps. Run them through a web interface.

ADD-ON PRODUCTS

ELECTROMAGNETICS

- AC/DC Module
- RF Module
- Wave Optics Module
- Ray Optics Module
- Plasma Module
- Semiconductor Module

FLUID & HEAT

- CFD Module
  - Mixer Module
- Polymer Flow Module
- Microfluidics Modul
- Porous Media Flow M
- Subsurface Flow Mo
- 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 Reaction Engineering 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

INTERFACING

- LiveLink™ *for* MATLAB®
- LiveLink™ *for* Simulink®
- LiveLink™ *for* Excel®
- CAD Import Module
- Design Module
- D Import Module
- Link™ *for* SOLIDWORKS®
- Link™ *for* Inventor®
- LiveLink™ *for* AutoCAD®
- LiveLink™ *for* Revit®
- LiveLink™ *for* PTC Creo Parametric™
- LiveLink™ *for* Solid Edge®
- File Import *for* CATIA® V5

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™

Host and administrate your simulation apps. Run them through a web interface.

ADD-ON PRODUCTS

ELECTROMAGNETICS

- AC/DC Module
- RF Module
- Wave Optics Module
- Ray Optics Module
- Plasma Module
- Semiconductor Module

FLUID & HEAT

- 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

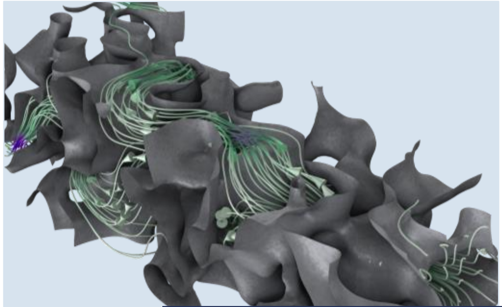
MULTIPURPOSE

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

INTERFACING

- LiveLink™ *for* MATLAB®
- LiveLink™ *for* Simulink®
- LiveLink™ *for* Excel®
- CAD Import Module
- Design Module
- ECAD Import Module
- LiveLink™ *for* SOLIDWORKS®
- LiveLink™ *for* Inventor®
- LiveLink™ *for* AutoCAD®
- LiveLink™ *for* Revit®
- LiveLink™ *for* PTC Creo Parametric™
- LiveLink™ *for* Solid Edge®
- File Import *for* CATIA® V5

Fluid Flow in Porous Media

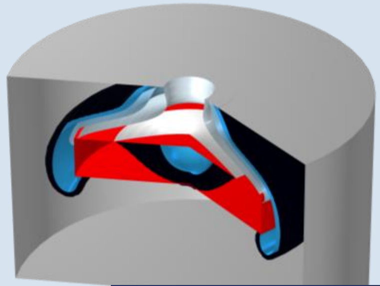


Single Phase Flow

Laminar or Creeping flow

Darcy‘s law, Richards‘ Equation

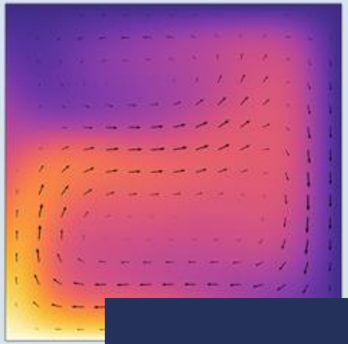
Brinkman equations (Laminar, Turbulent)



Multiphase Flow

Multiphase transport

Front tracking with Level-set Brinkman



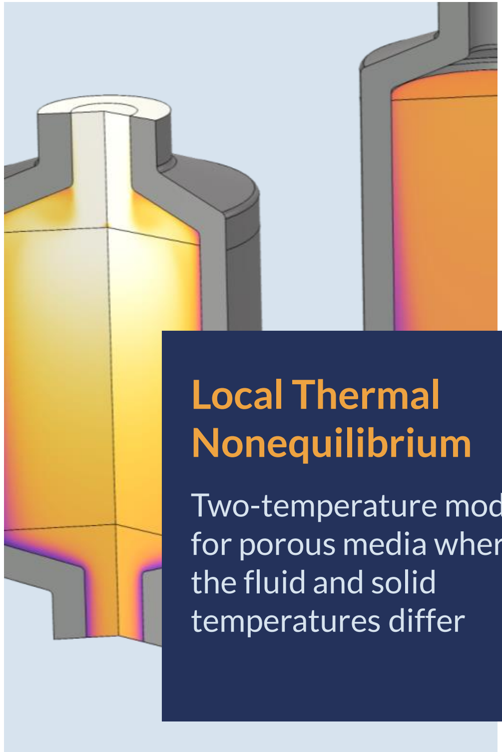
Nonisothermal Flow

Predefined coupling of Brinkman equations and heat transfer in porous media

Heat Transfer in Porous Media

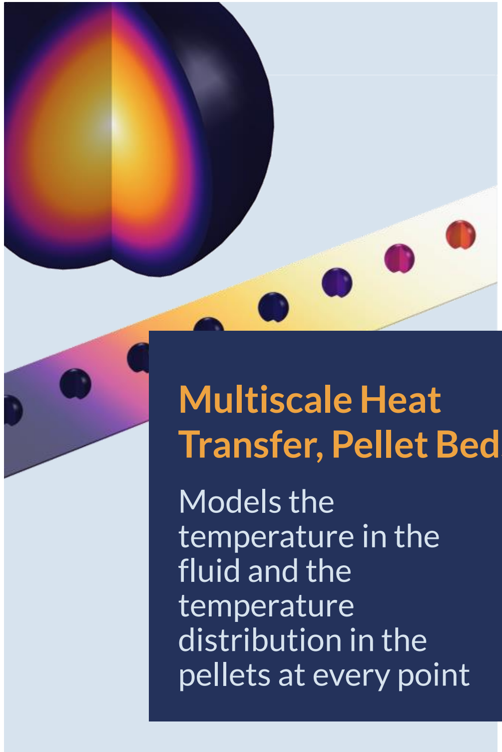
Local Thermal Equilibrium

Homogenized porous media; predefined models for effective thermal conductivity



Local Thermal Nonequilibrium

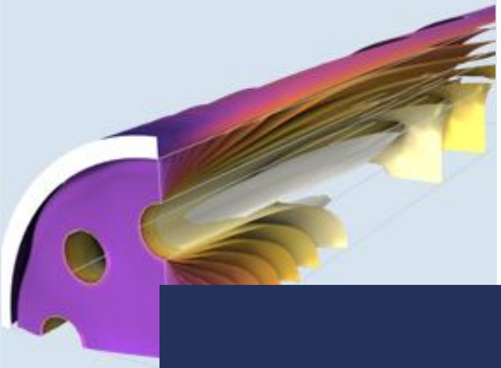
Two-temperature model for porous media where the fluid and solid temperatures differ



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

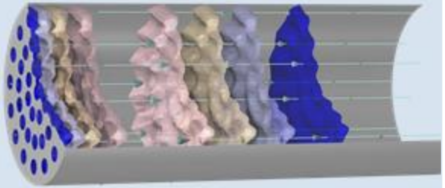


Solute

Diffusion, conduction, and dispersion models

Adsorption isotherms

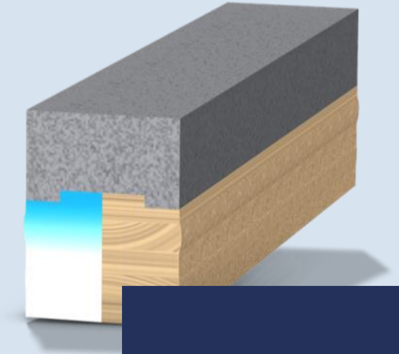
Volatilization



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.

COMSOL

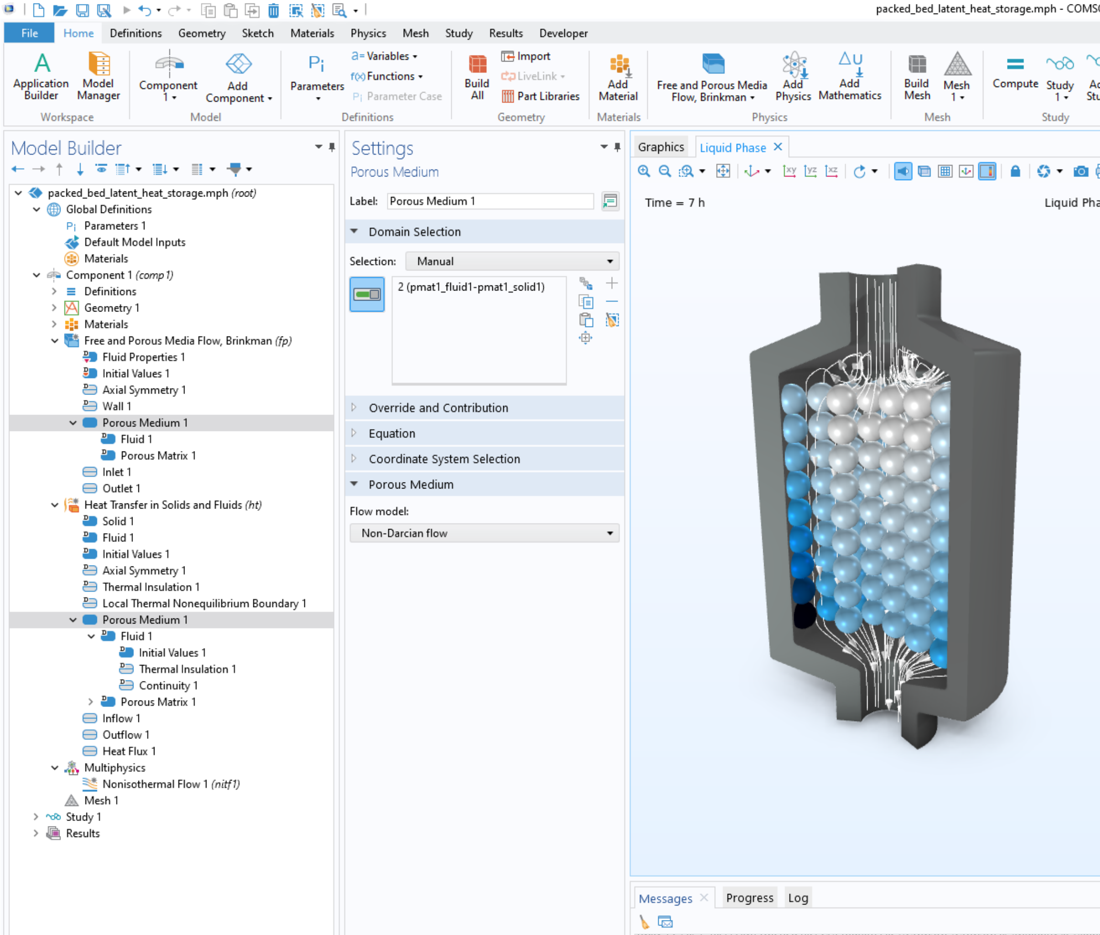
Modelling Porous Materials

Porous Medium

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

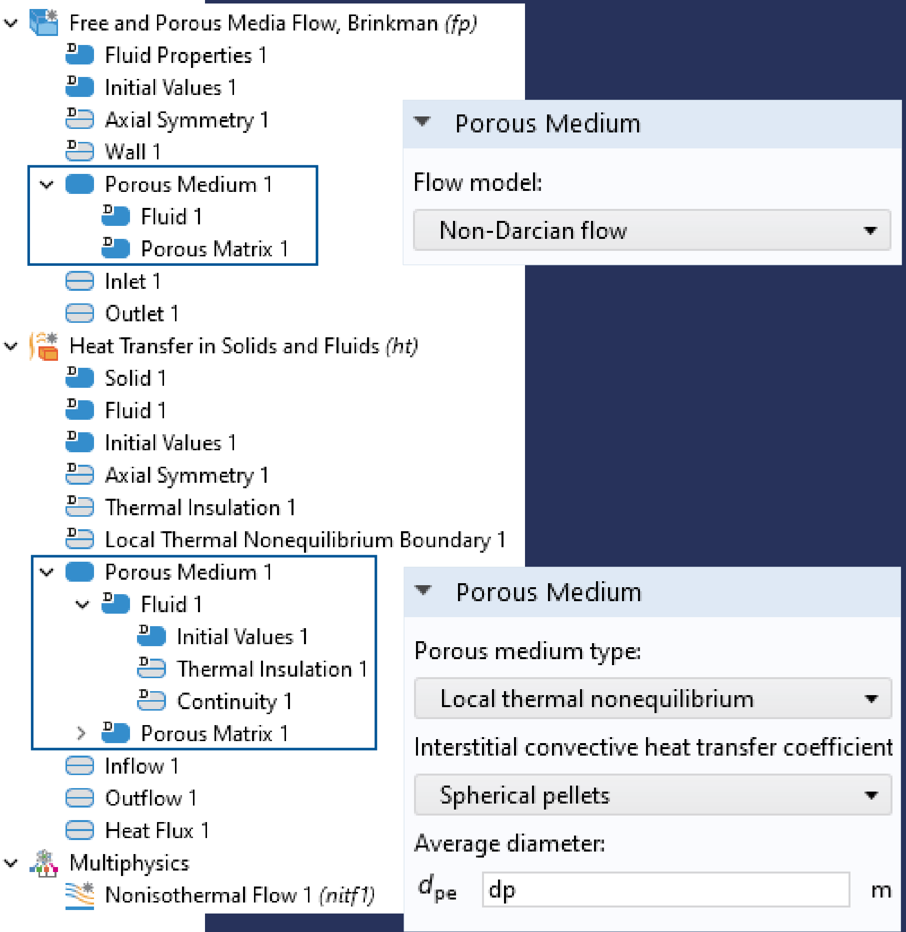
Porous Material

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



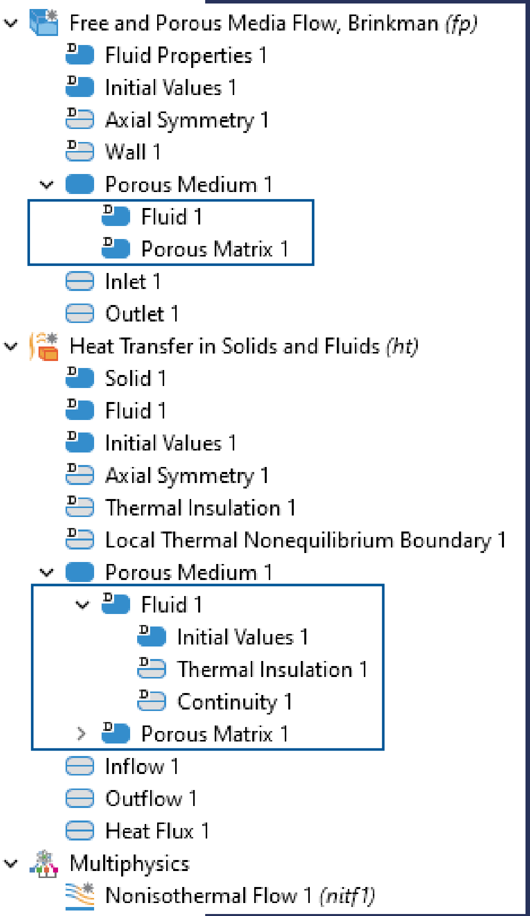
Porous Medium

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



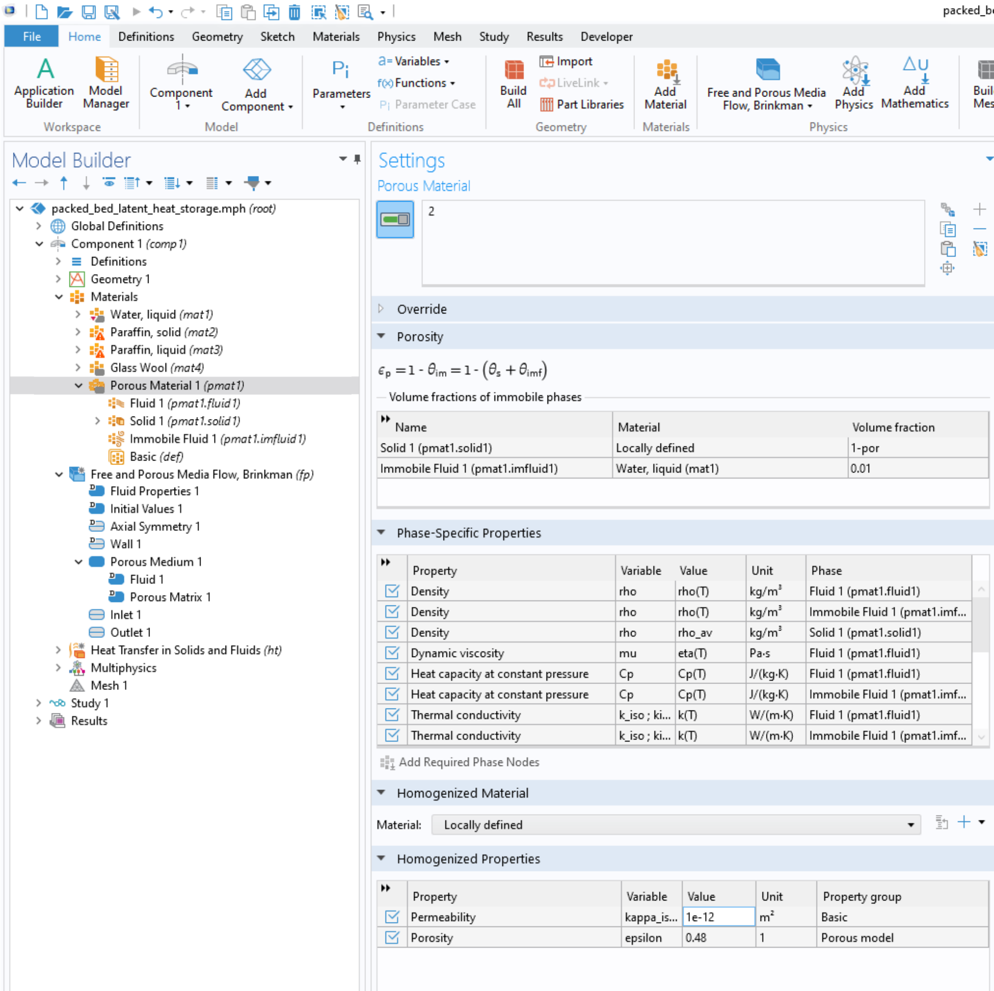
Porous Medium

- 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



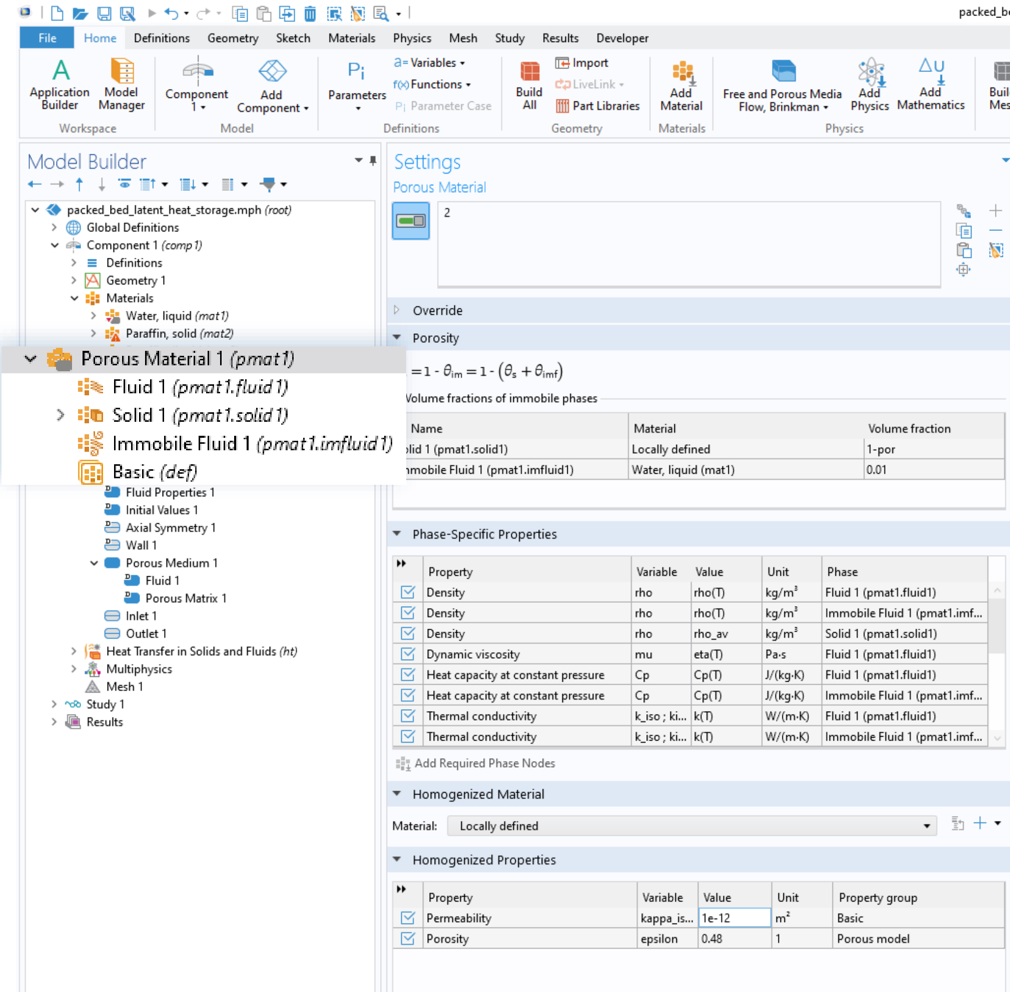
Porous Material

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



Porous Material

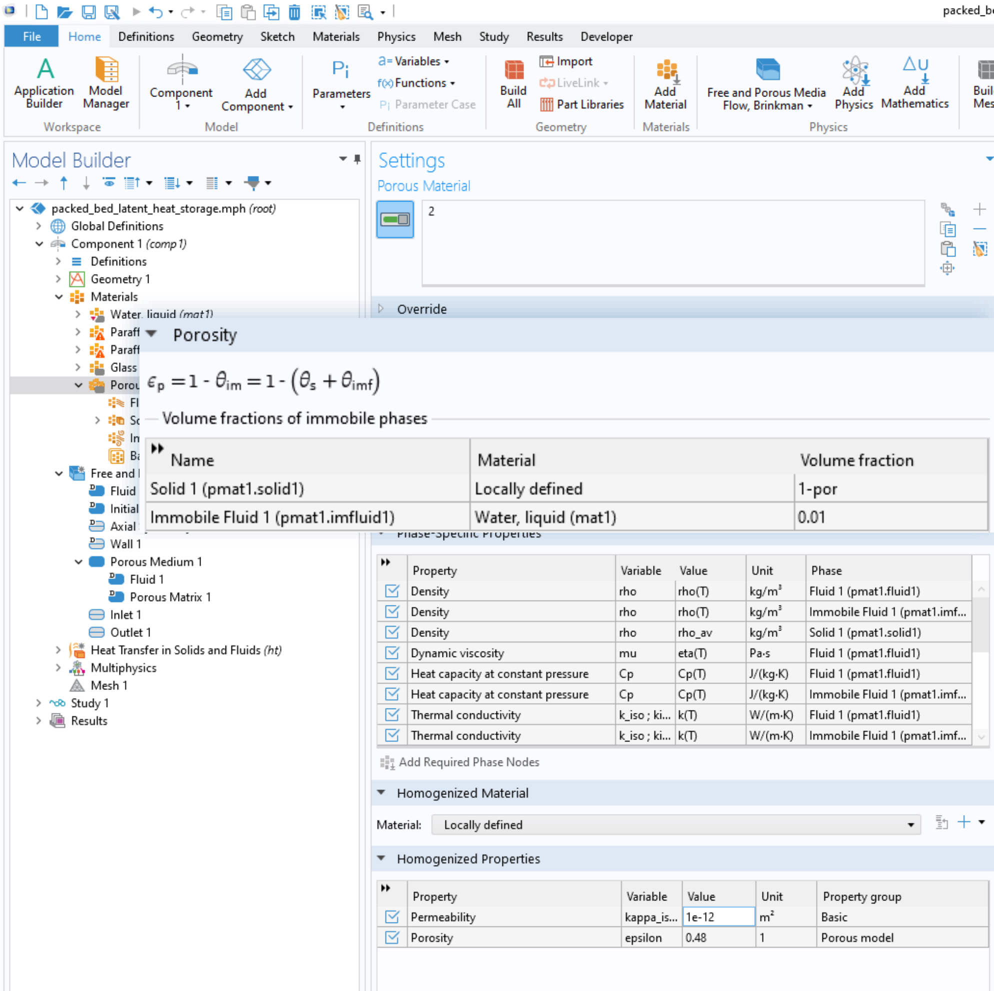
Which phases require definition is dictated by the physics involved, and the porous material detects what needs to be specified.



COMSOL

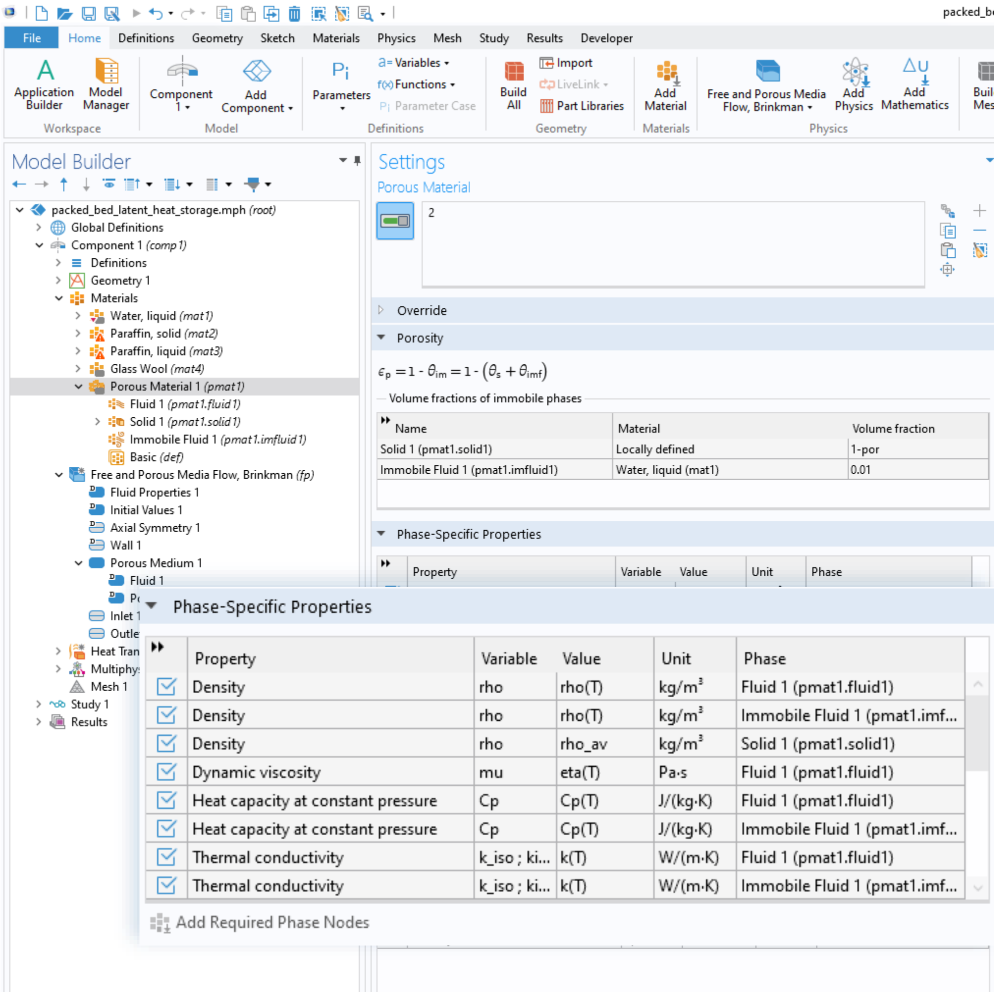
Porous Material

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



Porous Material

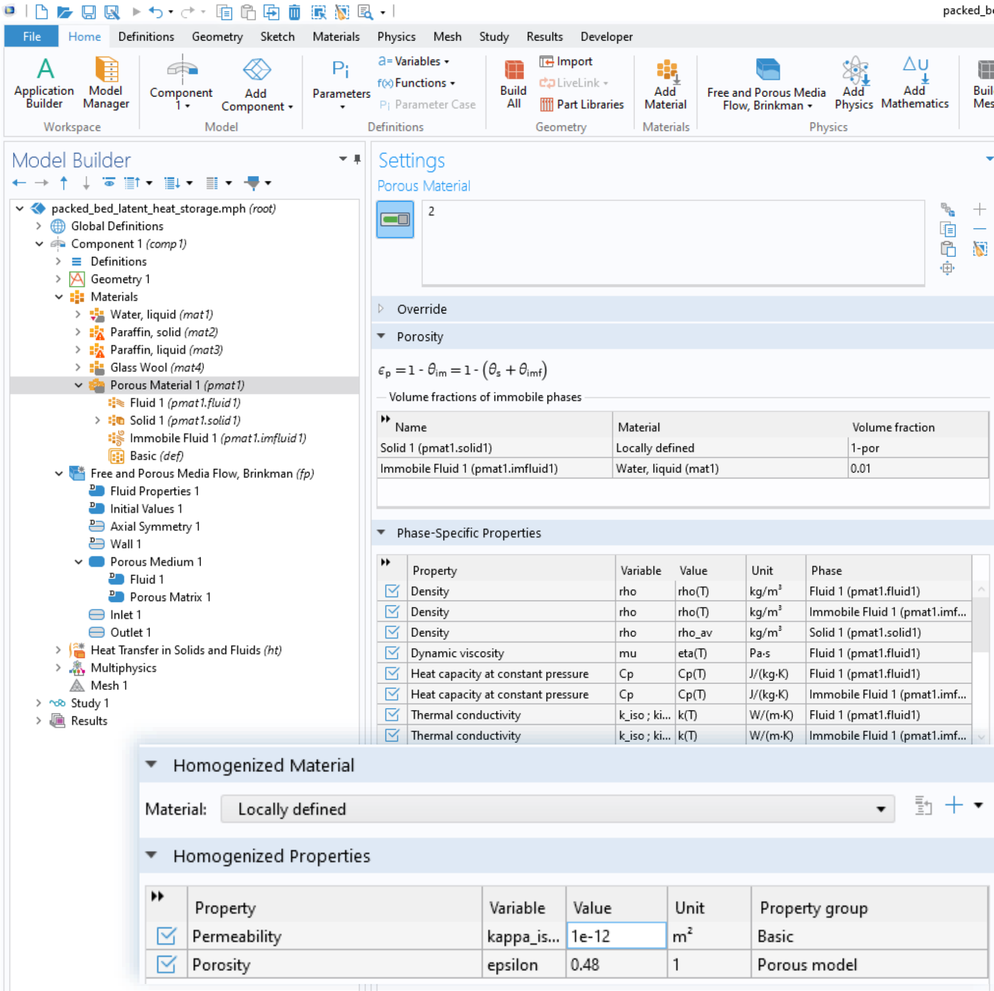
Phase-Specific Properties such as for the solid, fluid, or immobile fluid phase are defined in the corresponding subnode of the Porous Material.



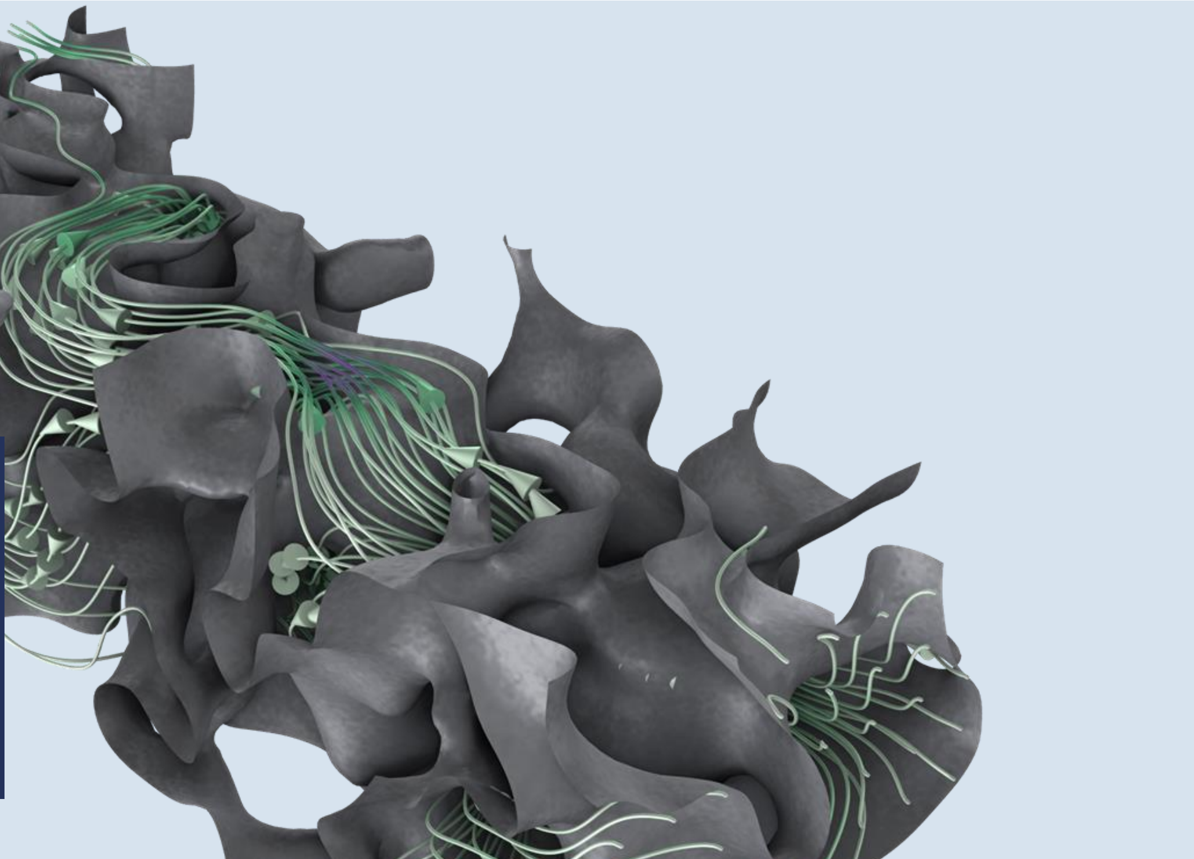
Porous Material

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.



COMSOL

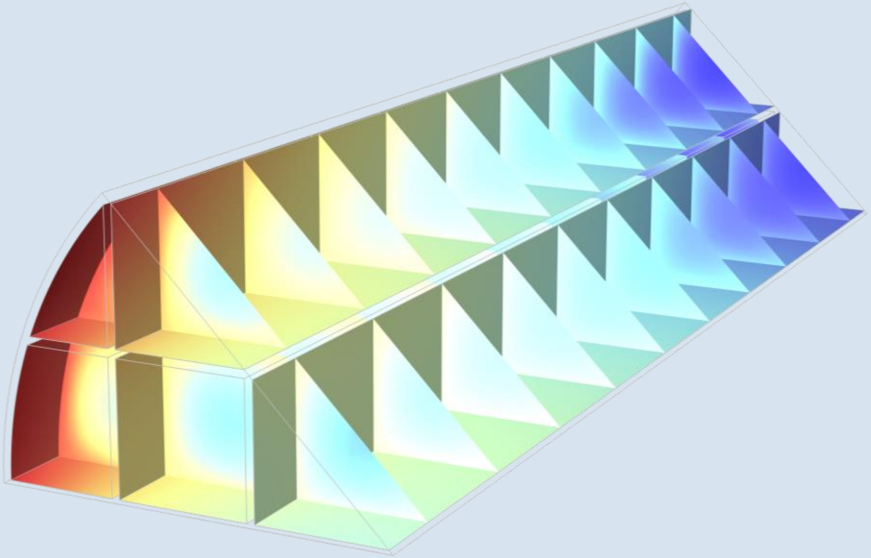


THE FLUID FLOW INTERFACES

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

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

Applications

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

Permeability Models

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

Storage Models

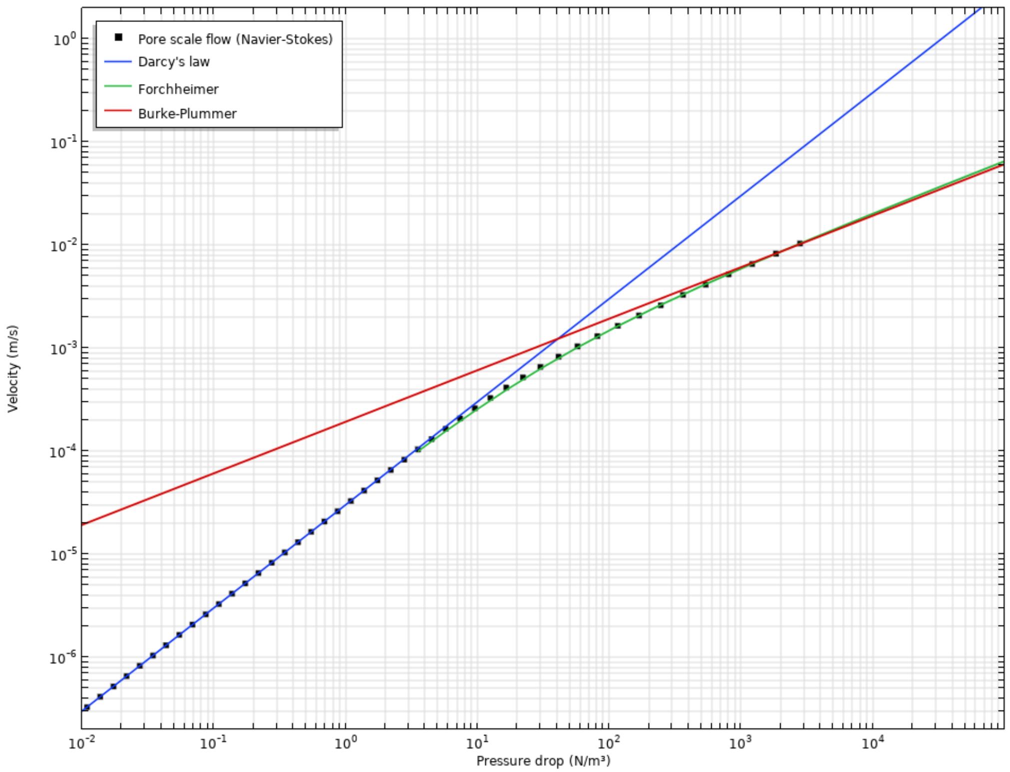
Include different storage models to account for water absorbed or released due to changes in hydraulic head

Non-Darcian Flow

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

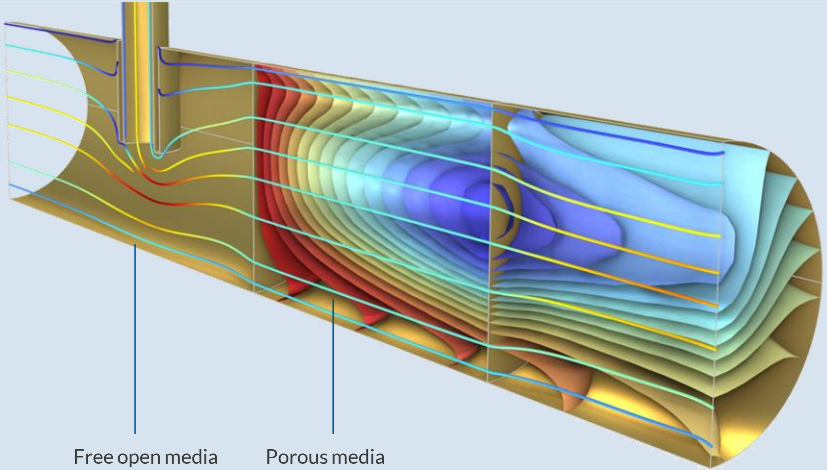
$$\nabla p = -\frac{\mu}{\kappa}\mathbf{u} - \beta\rho|\mathbf{u}|\mathbf{u}$$

  - Forchheimer and Ergun ($\mathrm{Re} < 1000$)
  - Burke–Plummer ($\mathrm{Re} > 1000$)
  - 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

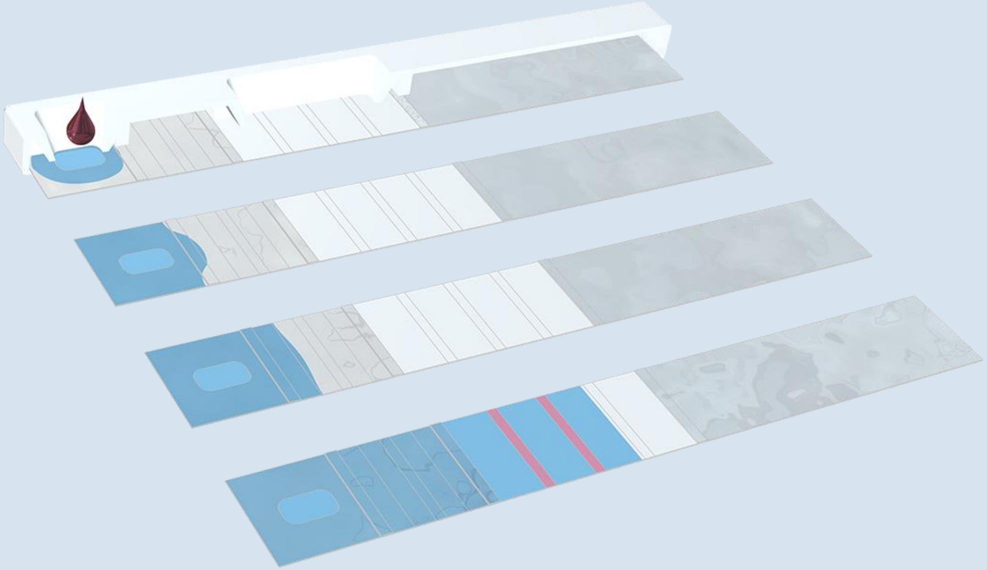
Turbulence

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

COMSOL

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

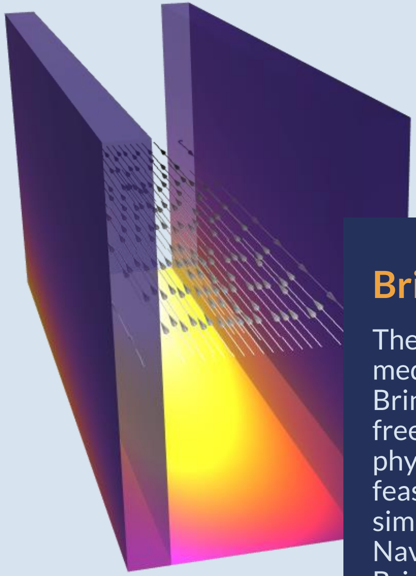
Retention Models

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

Storage Models

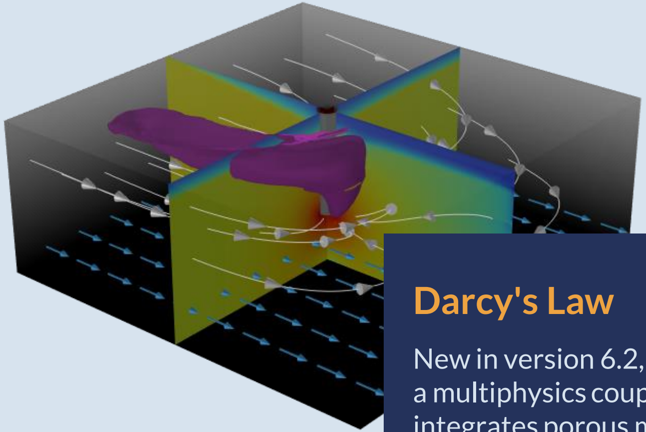
Account for storage of fluid using linearized or user-defined models or storage from liquid content

Free and Porous Media Flow



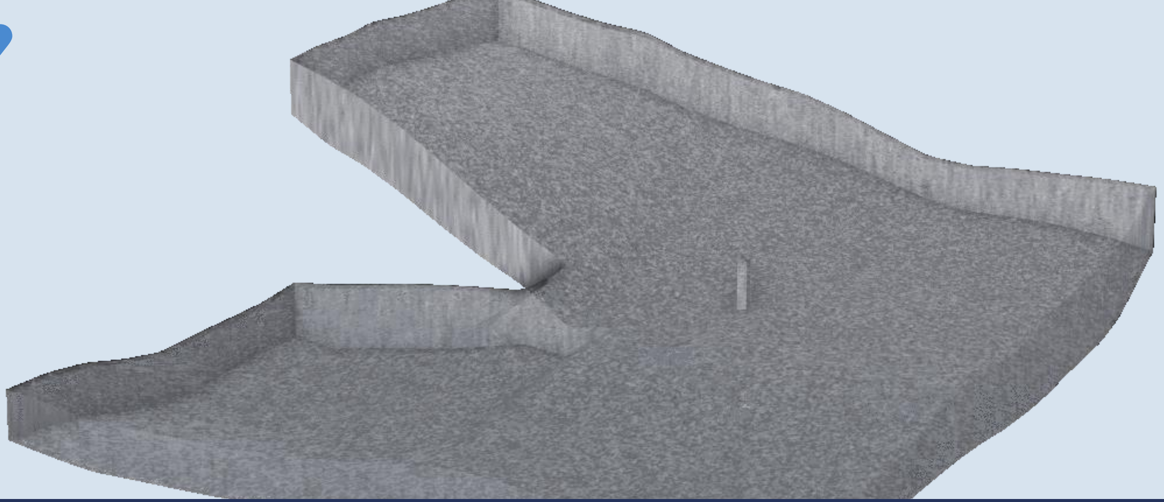
Brinkman Equations

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

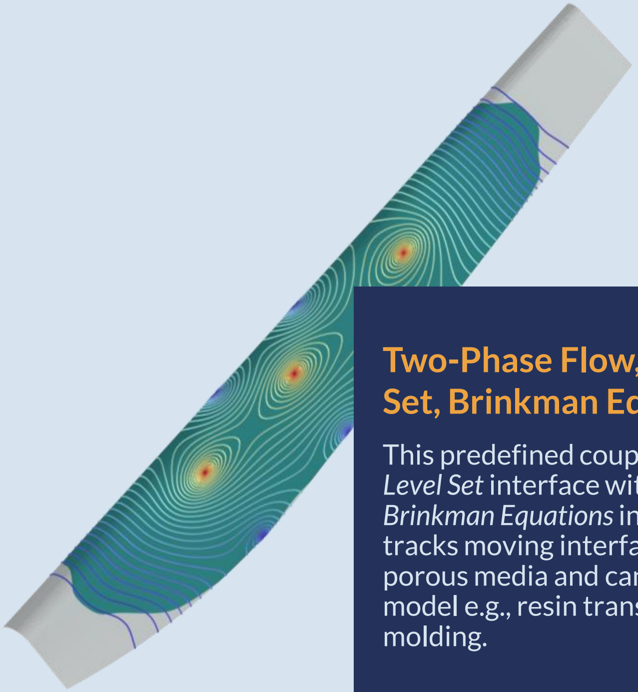
Applications

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

Challenges

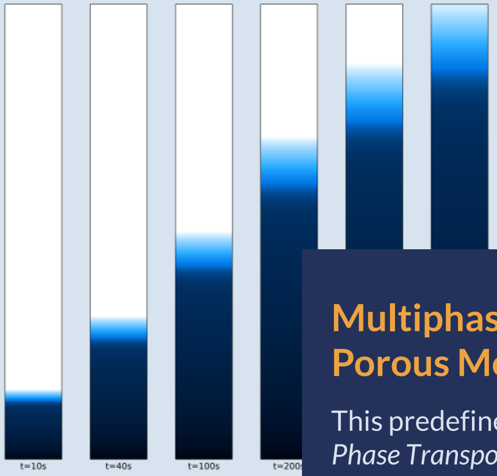
Complex phenomena due to interfacial tension, capillary pressure, and wettability, and phenomena like phase transitions and saturation changes

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.

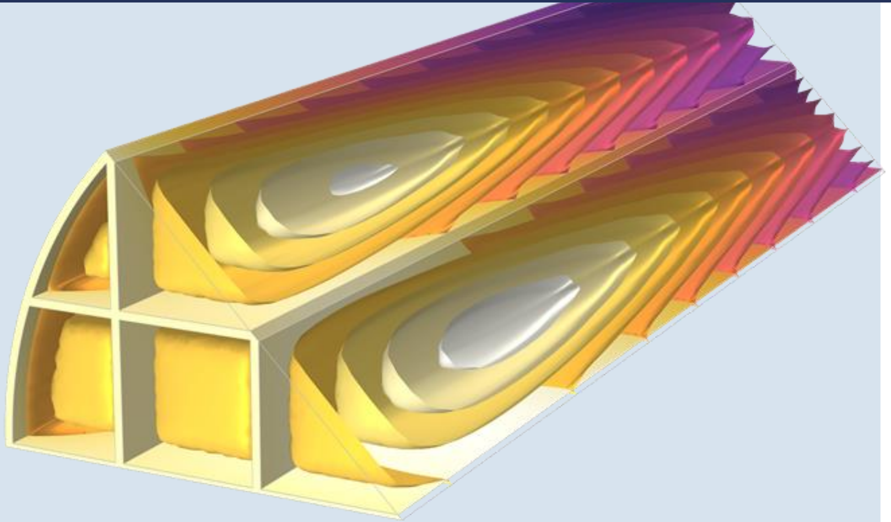


Multiphase Flow in Porous Media

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

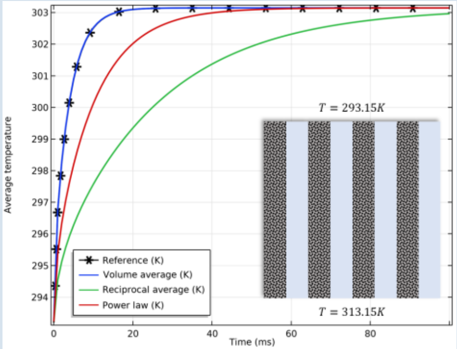
Effective values for material properties of different structures of porous materials, with up to five different immobile phases

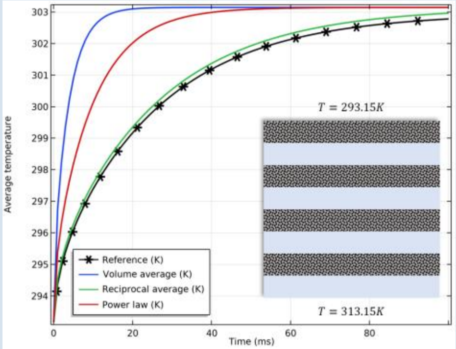
Thermal Dispersion

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

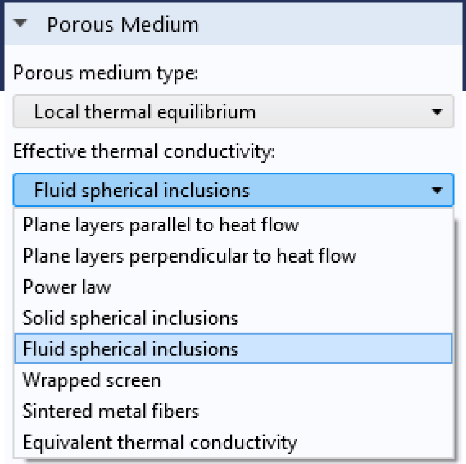
Geothermal Heating

Add contributions from radiogenic heat production and geothermal gradients





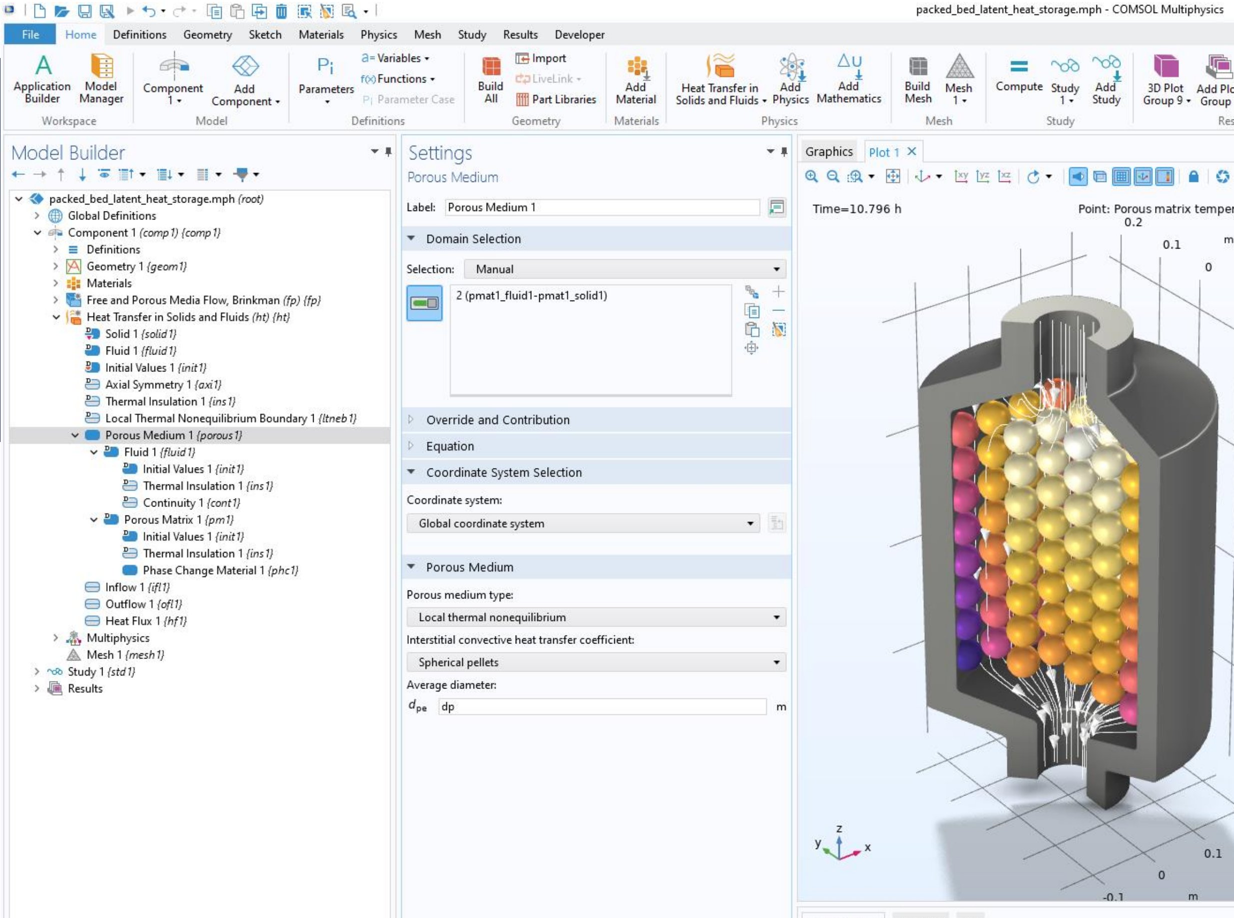
Local Thermal Equilibrium



- 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

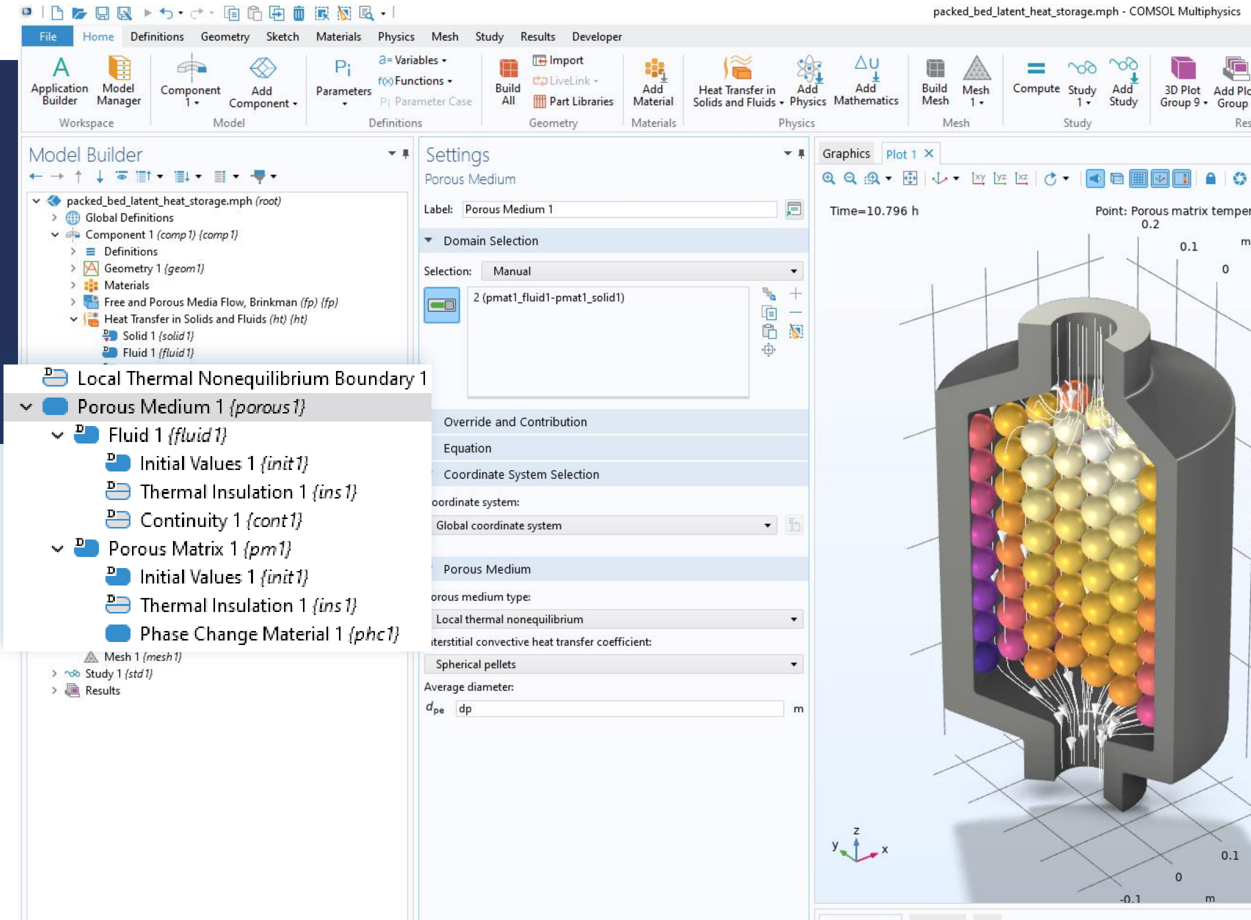
- Solid and fluid temperature are not in local equilibrium
- Temperature differences can be substantial for fast nonisothermal flows, phase change, or on short time scales



COMSOL

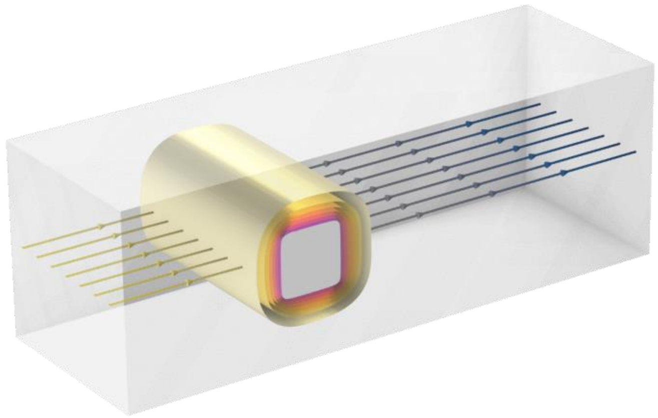
Local Thermal Nonequilibrium

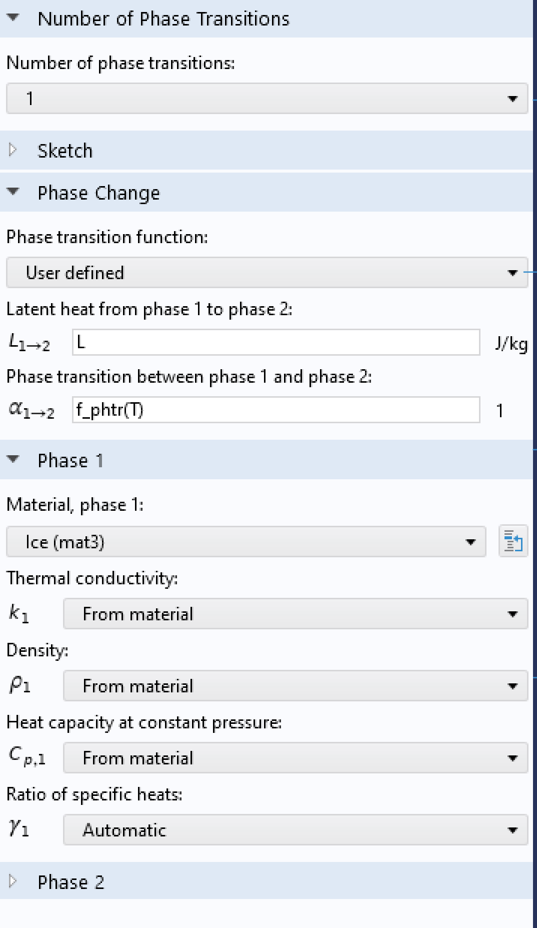
- Fluid and Solid each have default boundary conditions (interaction with adjacent domains) and initial values.
- Additional subnodes are available for each phase.
- Local Thermal Nonequilibrium Boundary for two-temperature boundaries



Phase Change in Porous Media

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



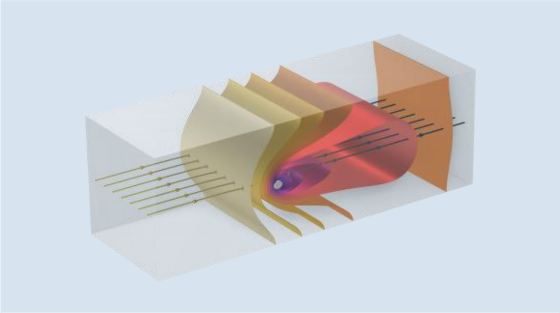


Number of phase transitions

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

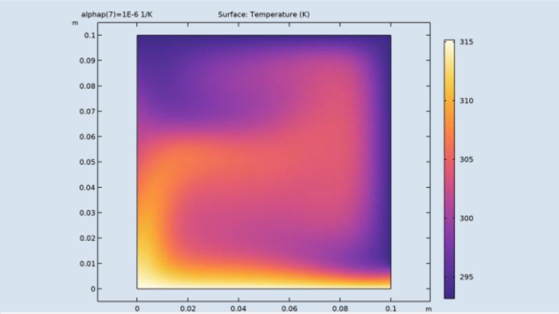
Set up material properties for each phase

Nonisothermal Flow



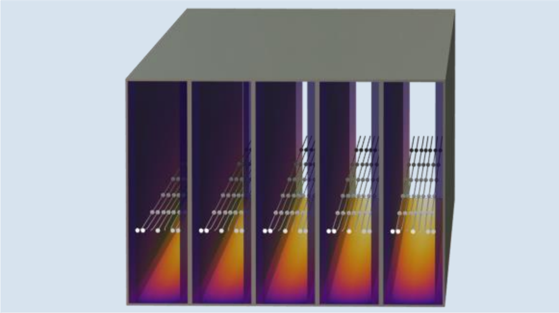
Material Properties

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



Free Convection

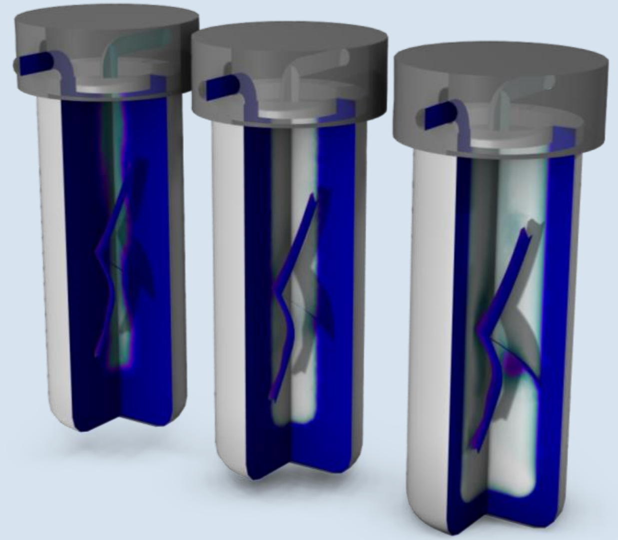
Buoyancy effects due to temperature gradients lead to density differences, driving natural convection. Use the Boussinesq approximation method to simplify the density variations in the buoyancy term



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

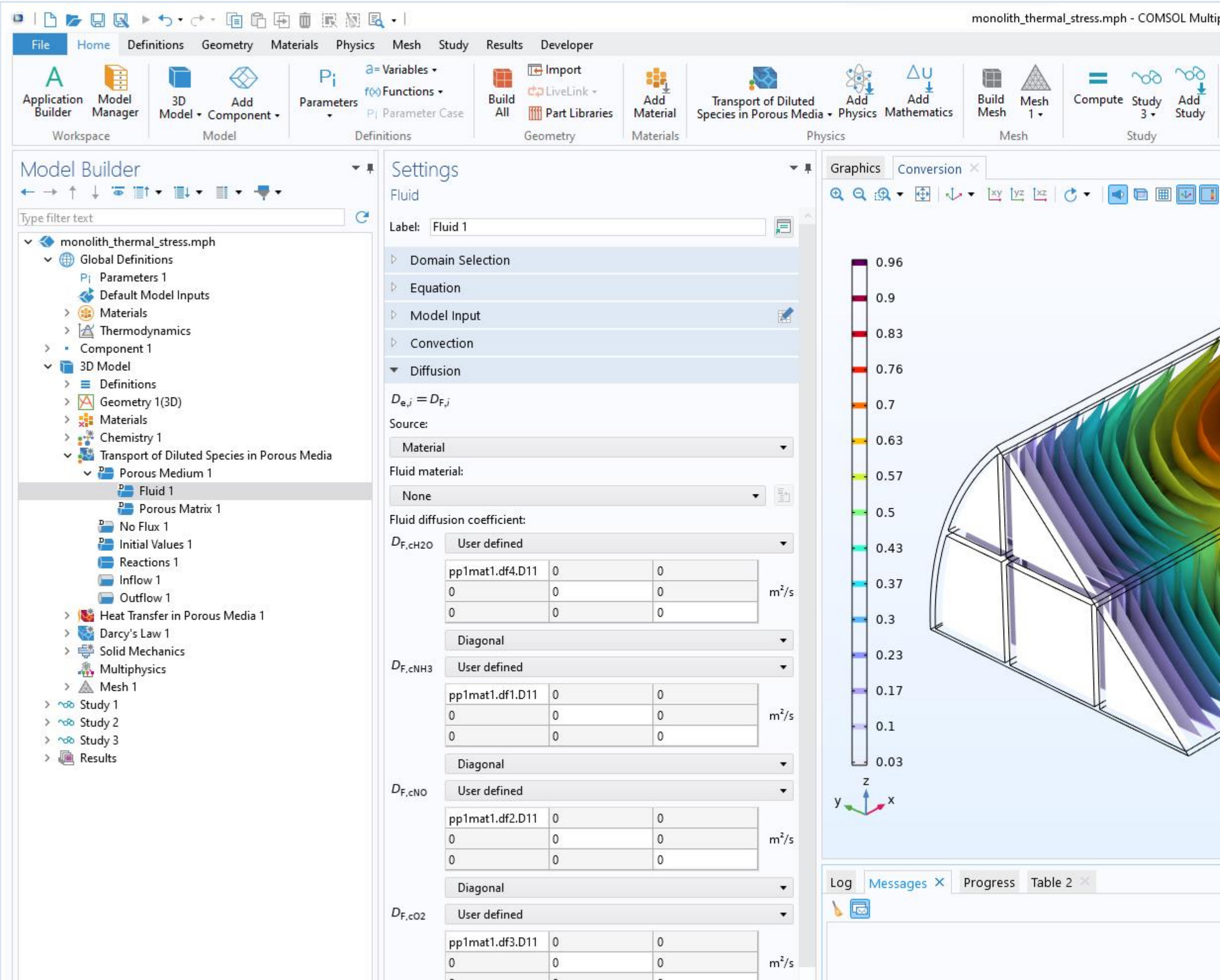
Dispersion

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

COMSOL

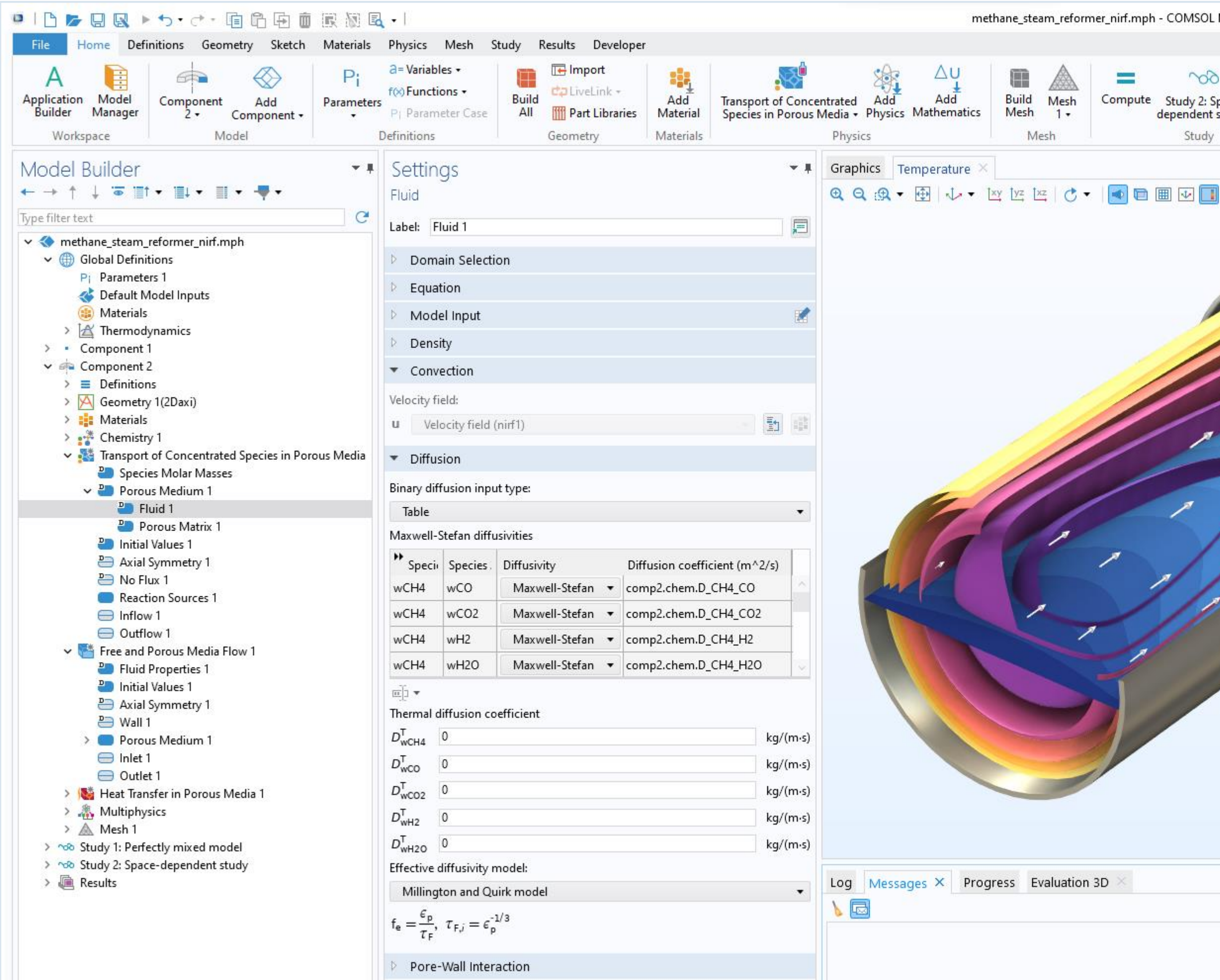
Transport of Diluted Species in Porous Media

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

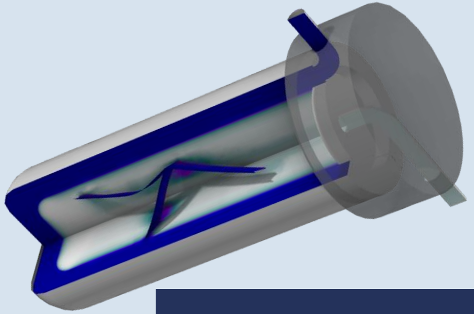


Transport of Concentrated Species in Porous Media

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

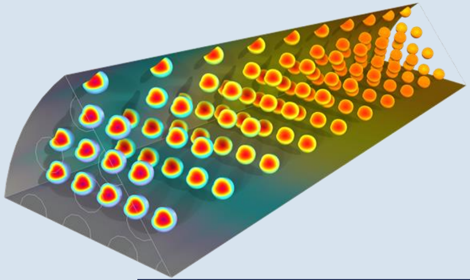


Porous Medium Types



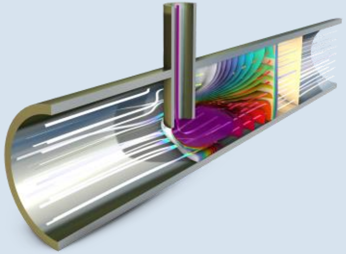
Porous Medium

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



Packed Bed

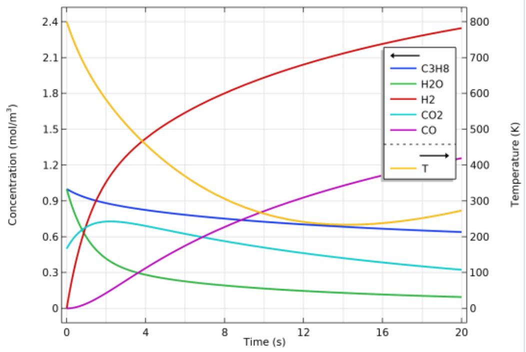
Porous catalytic particles in a fixed bed reactor. Models transport inside particles as well as in the bed macropores.



Porous Catalyst

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

Chemical Reaction Engineering Module: Modeling Strategy



Perfectly Mixed System

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

Species

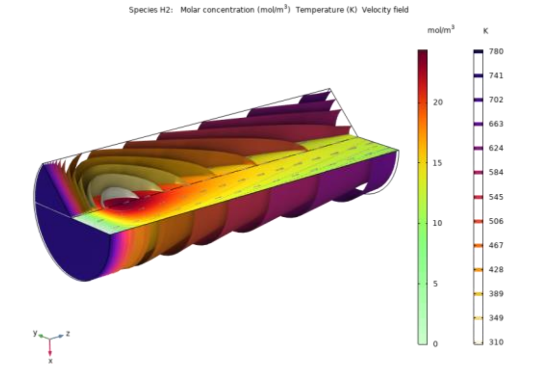
Name	CAS	Chemical formula	Database
carbon dioxide	124-38-9	CO2	COMSOL
carbon monoxide	630-08-0	CO	COMSOL
hydrogen	1333-74-0	H2	COMSOL
propane	74-98-6	C3H8	COMSOL
water	7732-18-5	H2O	COMSOL

Phases

Name	State
Gas	Vapor

Thermodynamic Properties

- Add a thermodynamic system
- Add compounds
- Match species

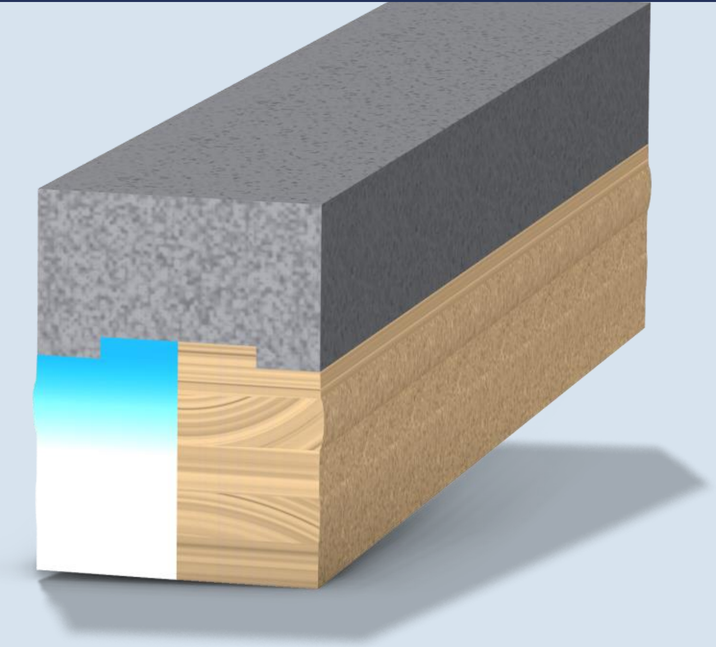


Generate Space-Dependent Model

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

COMSOL

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.

Characterization

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

Liquid Water

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

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.

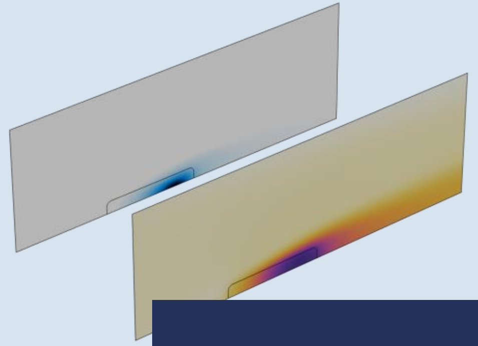
Moisture

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

Porous Matrix

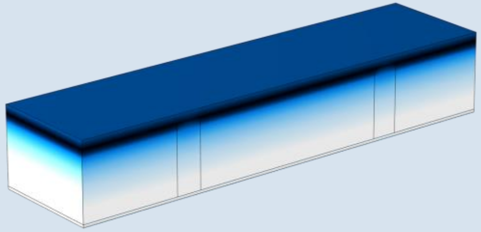
Liquid saturation and moisture content are dependent on the structure, varying with factors such as porosity, pore size distribution, and material composition.

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.

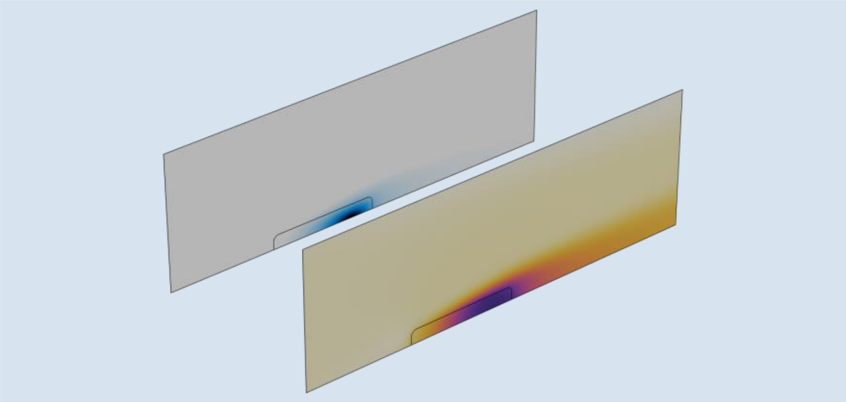
Specific equations for building materials under typical external conditions.

Porous Medium

Moisture transport in conjunction with deforming materials.

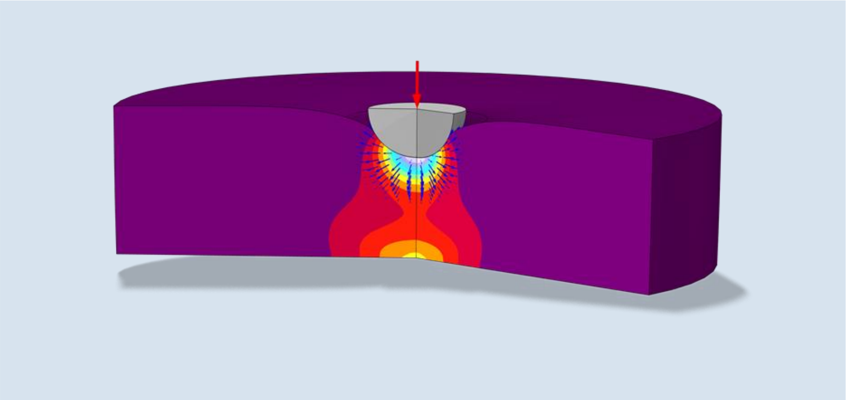
Accurate mass and energy conservation with large deformations.

Multiphysics Capabilities



Heat and Moisture

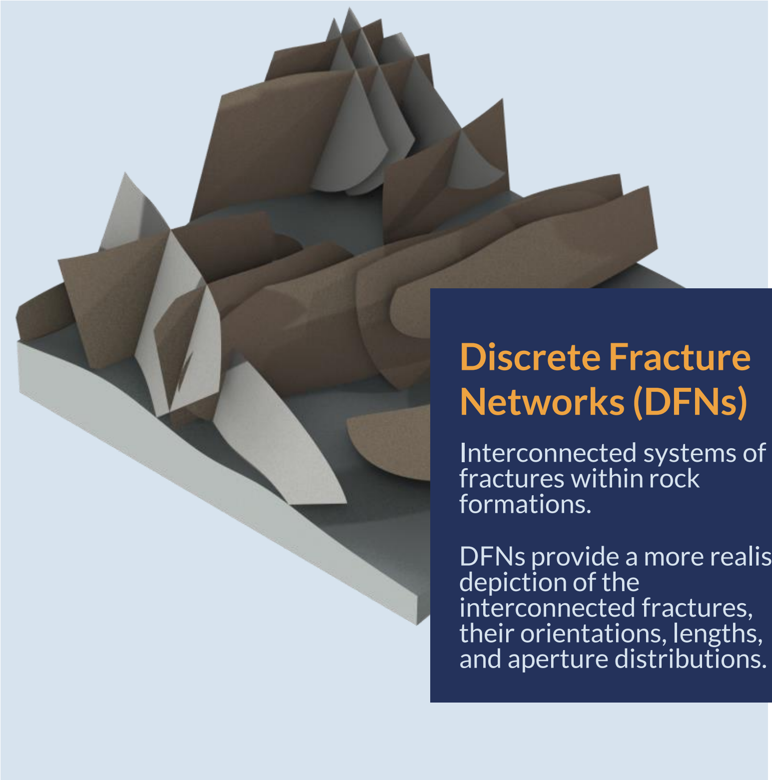
- Take into account heat and moisture storage, latent heat, and heat and moisture transport
- Relative humidity depends on temperature and pressure



Poroelasticity

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

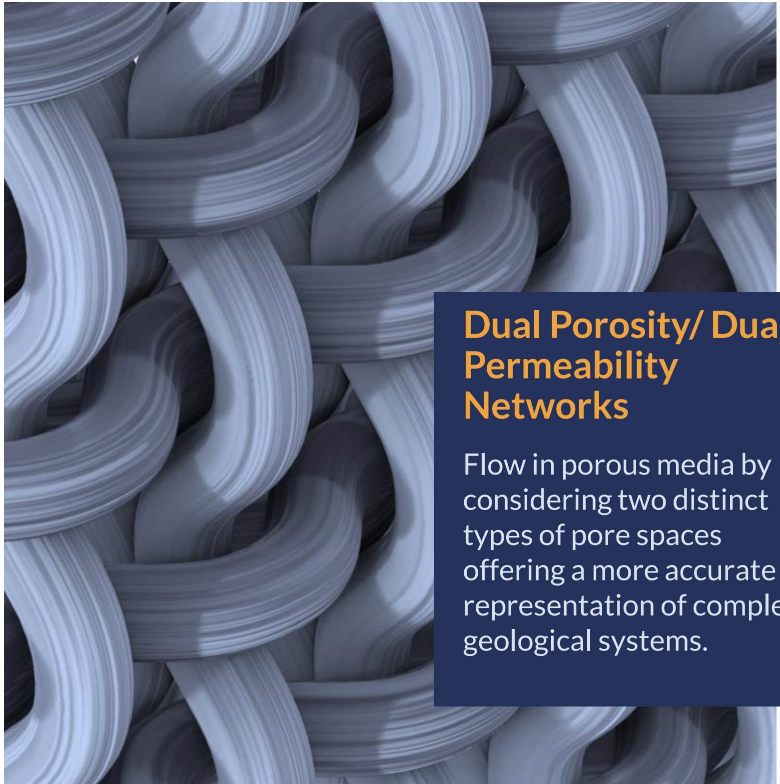
Complex Porous Materials



Discrete Fracture Networks (DFNs)

Interconnected systems of fractures within rock formations.

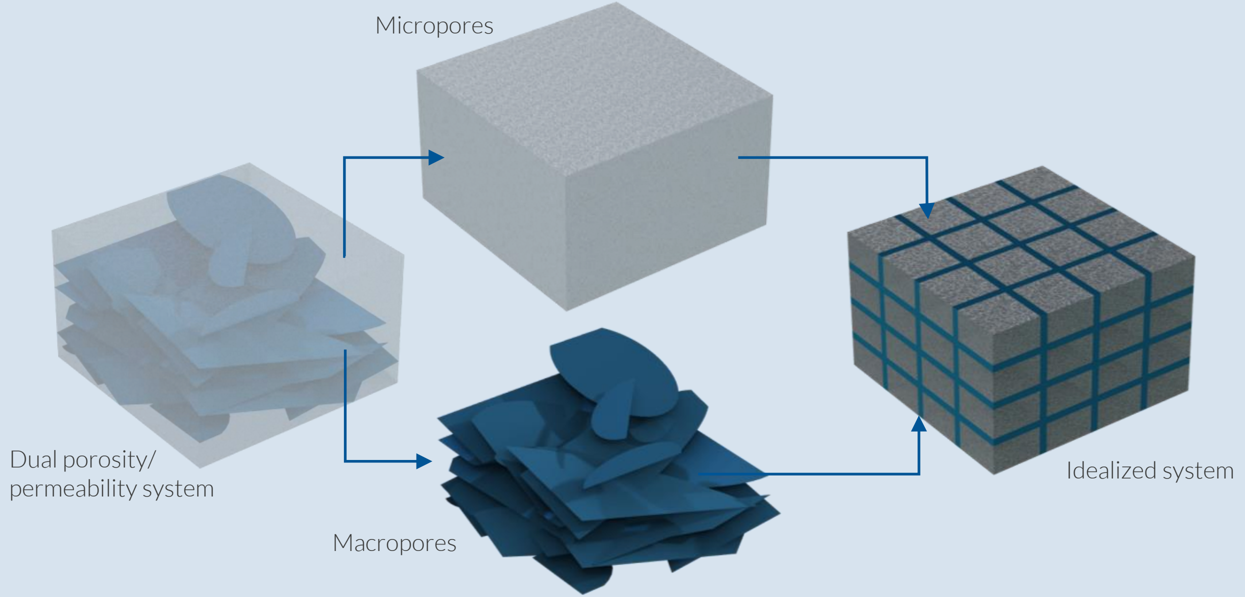
DFNs provide a more realistic depiction of the interconnected fractures, their orientations, lengths, and aperture distributions.



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

COMSOL

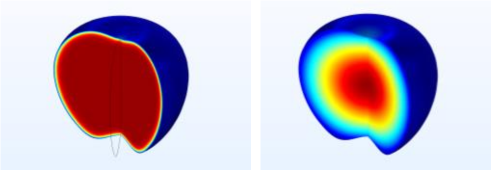
INNOVATION AT Empa

Forecasting Produce Shelf Life

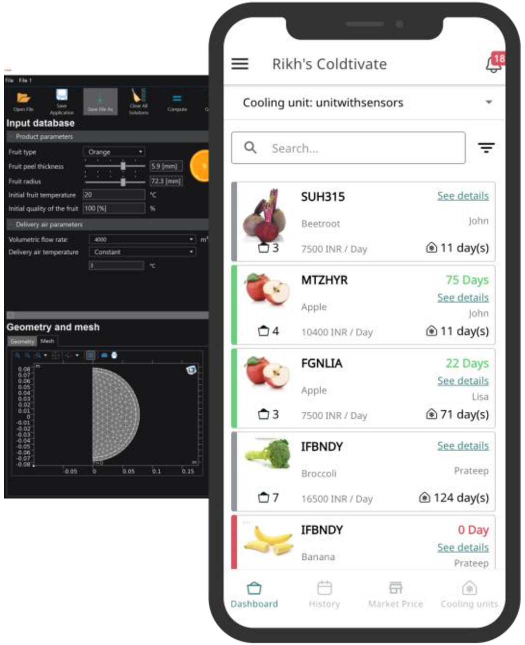
Each year, approximately one-third of the food produced for human consumption worldwide is lost or wasted. To optimize the use of refrigerated food storage in developing countries, farmers and traders need to be able to predict the shelf life of fresh fruits and vegetables.

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.

Forecasting Fruit Freshness with Simulation Apps

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

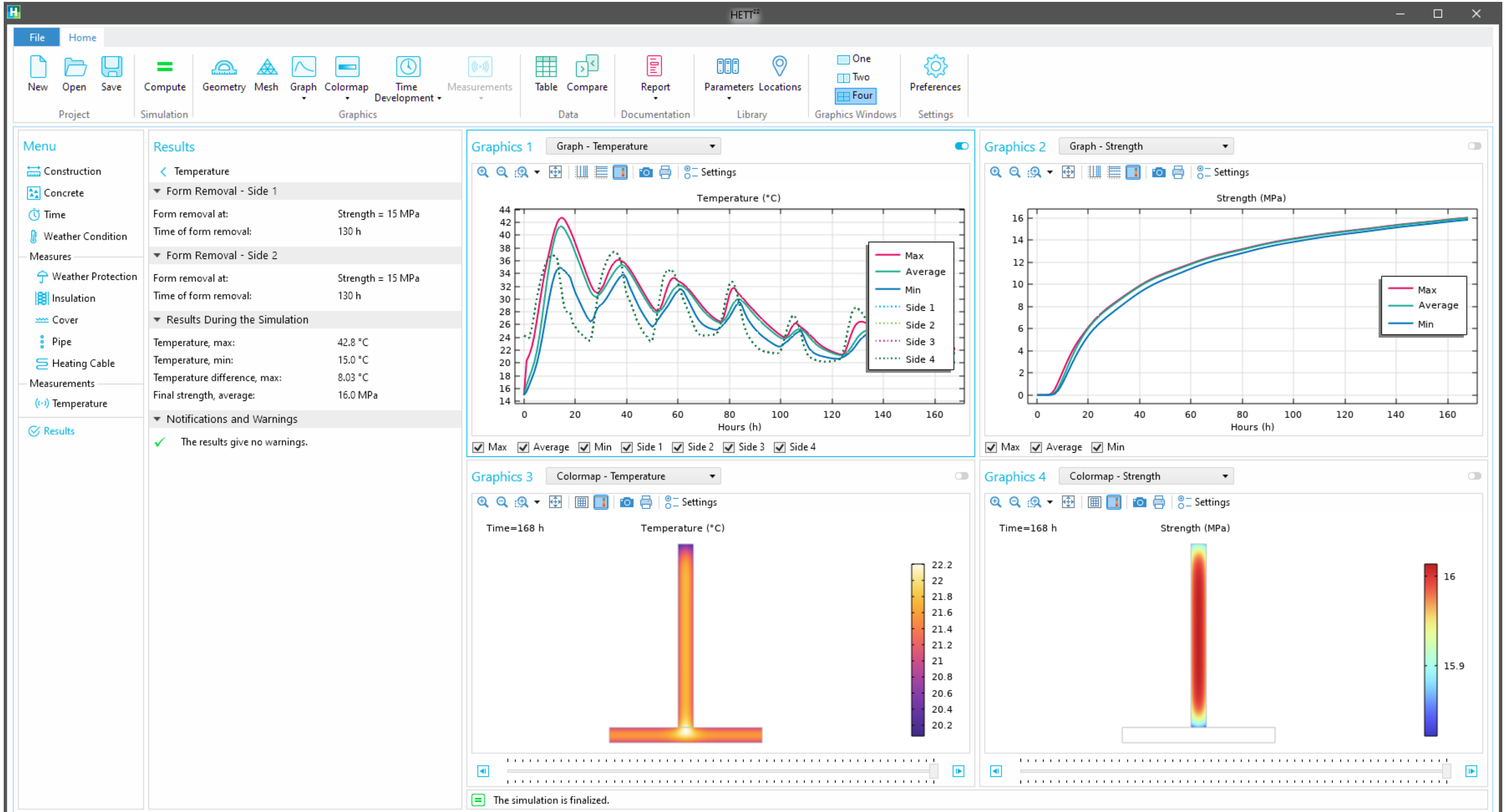
HETT^{22}

- 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

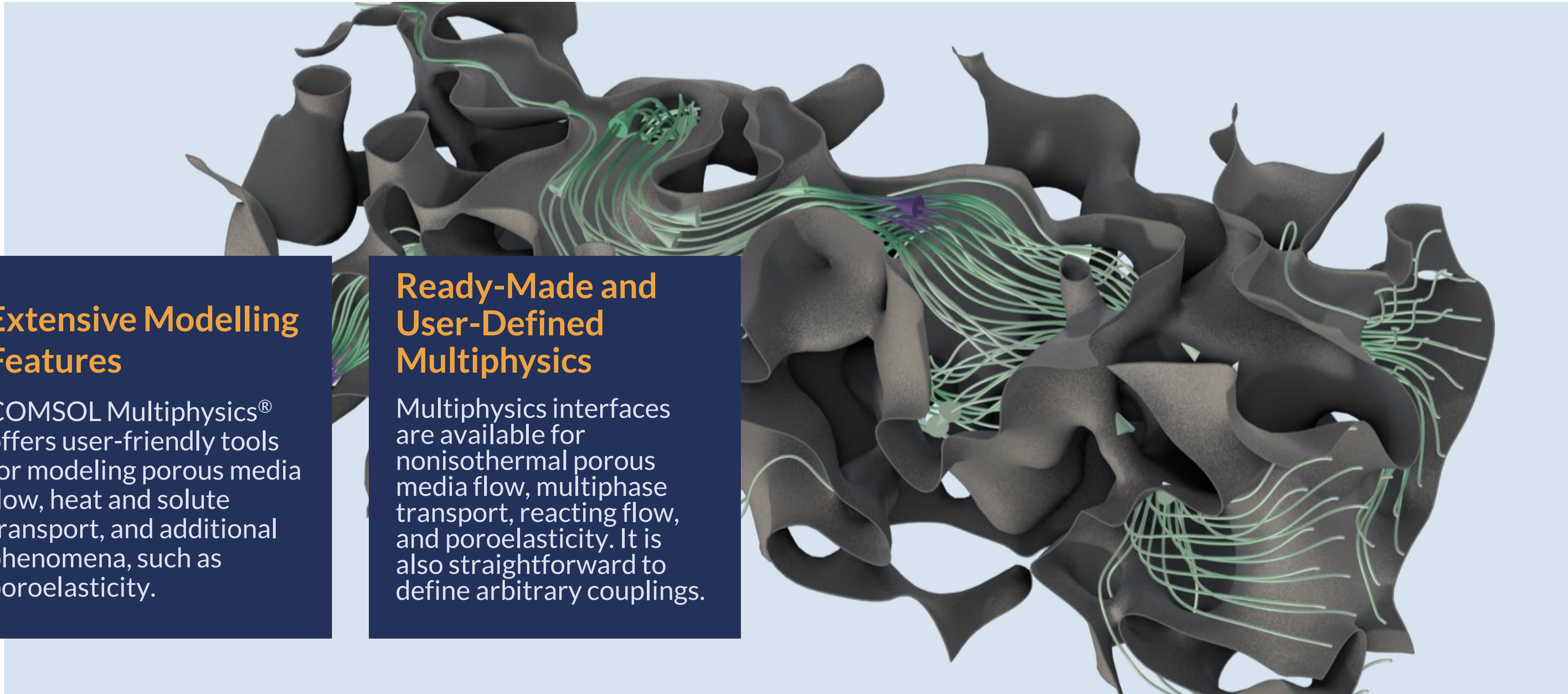
Developed by Deflexional AB
(COMSOL Certified Consultant)

deflexional

VISUALIZATION AND EVALUATION OF RESULTS



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.