Improve Carbon Capture, Utilization and Storage (CCUS) Projects with Subsurface Modeling & Simulation

October 7th, 2021

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DASSAULT SYSTEMES | The 3DEXPERIENCE® Company

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2

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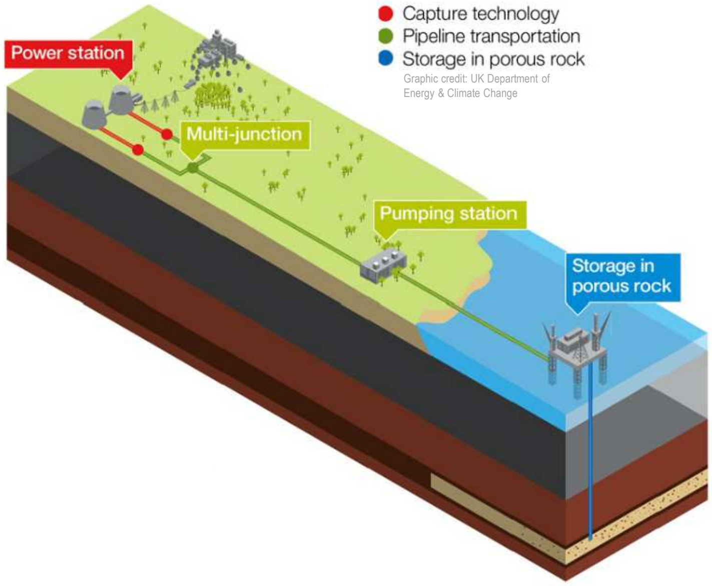

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The Purpose Is To Cool Planet Earth

4 Union of Concerned Scientists - Updated Aug 12, 2020

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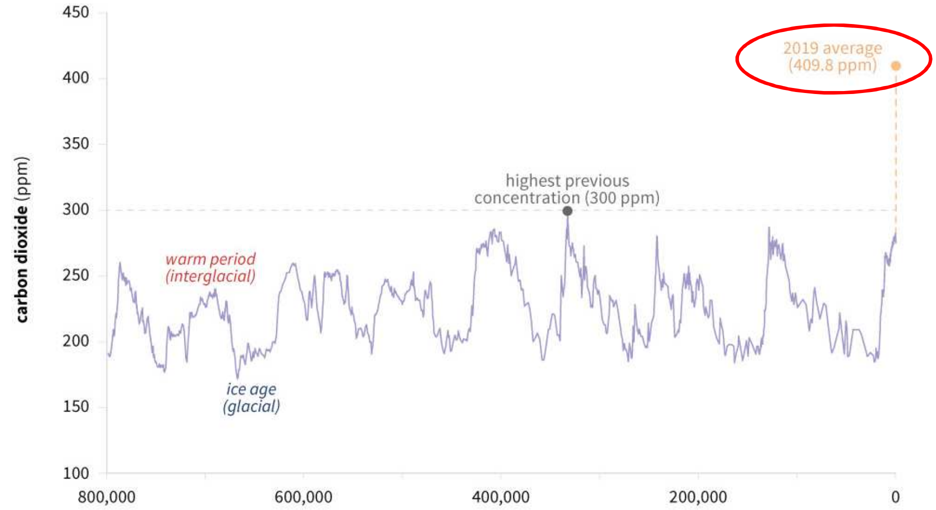
CO2 Over 800,000 Years Before Present



5 NOAA Climate.gov Data: NCEI

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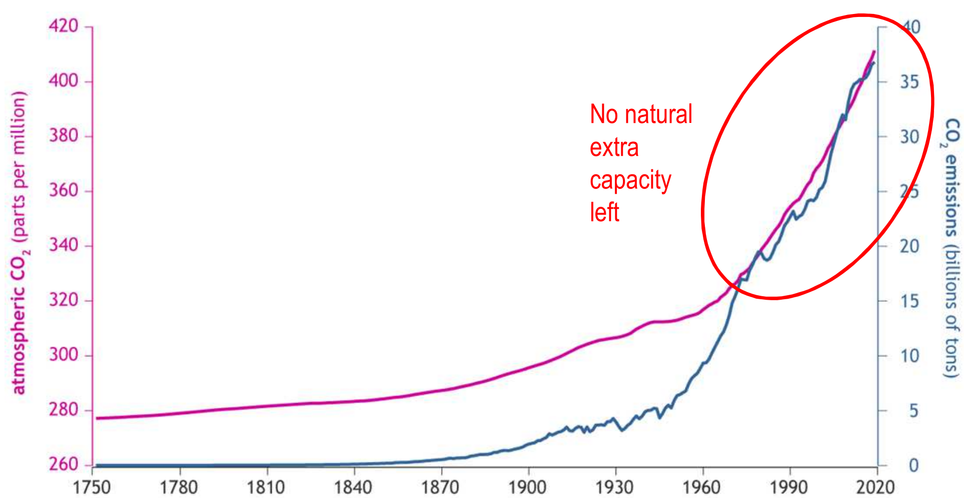
Atmosphere CO2 and Annual CO2 Emissions



6 NOAA Climate.gov Data: NOAA, ETHZ, Our World in Data

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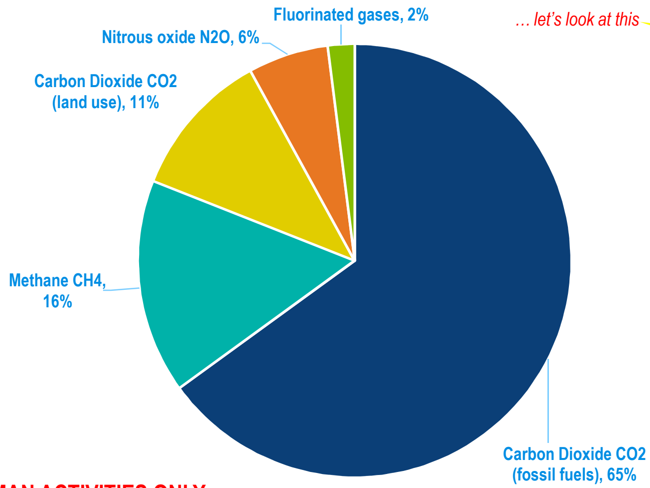
Global Greenhouse Gas Emissions By Gas



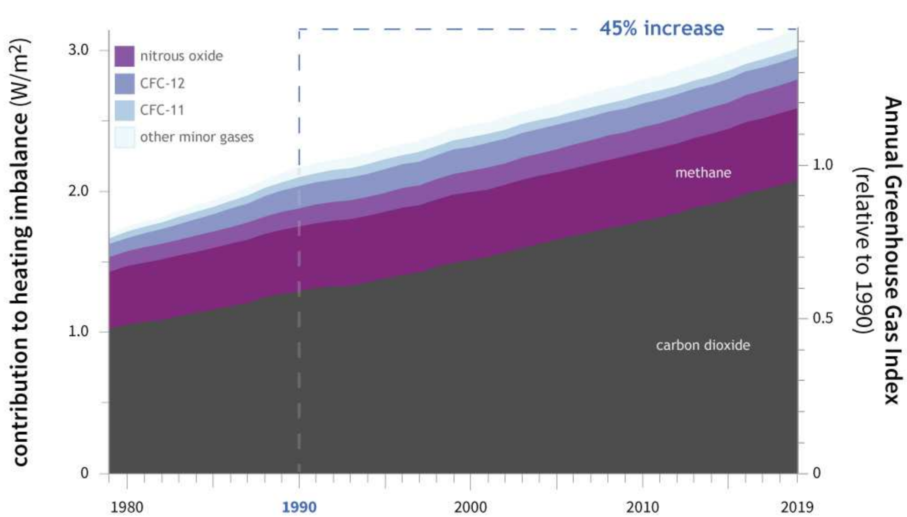
... let's look at this

Carbon dioxide (CO_2): Fossil fuel use is one of the primary source of CO_2. CO_2 can also be emitted from direct human-induced impacts on forestry and other land use, such as through deforestation, land clearing for agriculture, and degradation of soils. Likewise, land can also remove CO_2 from the atmosphere through reforestation, improvement of soils, and other activities.
Methane (CH_4): Agricultural activities, waste management, energy use, and biomass burning all contribute to CH_4 emissions.
Nitrous oxide (N_2O): Agricultural activities, such as fertilizer use, are the primary source of N_2O. Fossil fuel combustion also generates N_2O.
Fluorinated gases (F-gases): Industrial processes, refrigeration, and the use of a variety of consumer products contribute to emissions of F-gases, which include hydrofluorocarbons (HFCs), perfluorocarbons (PFCs), and sulfur hexafluoride (SF6).

HUMAN ACTIVITIES ONLY

7 EPA – Data from 2010

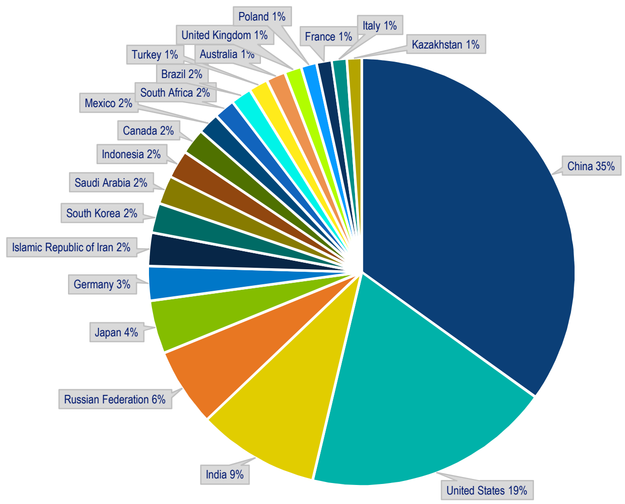
Greenhouse Gas Combined Heating Influence



8 NOAA Climate.gov Data: ESRL

Geography: Where CO2 Happens?

**FUEL COMBUSTION ONLY
TOP 20 COUNTRIES**



Country	Metric Gigatons
China	10.06
United States	5.41
India	2.65
Russian Federation	1.71
Japan	1.16
Germany	0.75
Islamic Republic of Iran	0.72
South Korea	0.65
Saudi Arabia	0.62
Indonesia	0.61
Canada	0.56
Mexico	0.47
South Africa	0.46
Brazil	0.45
Turkey	0.42
Australia	0.42
United Kingdom	0.37
Poland	0.34
France	0.33
Italy	0.33
Kazakhstan	0.32

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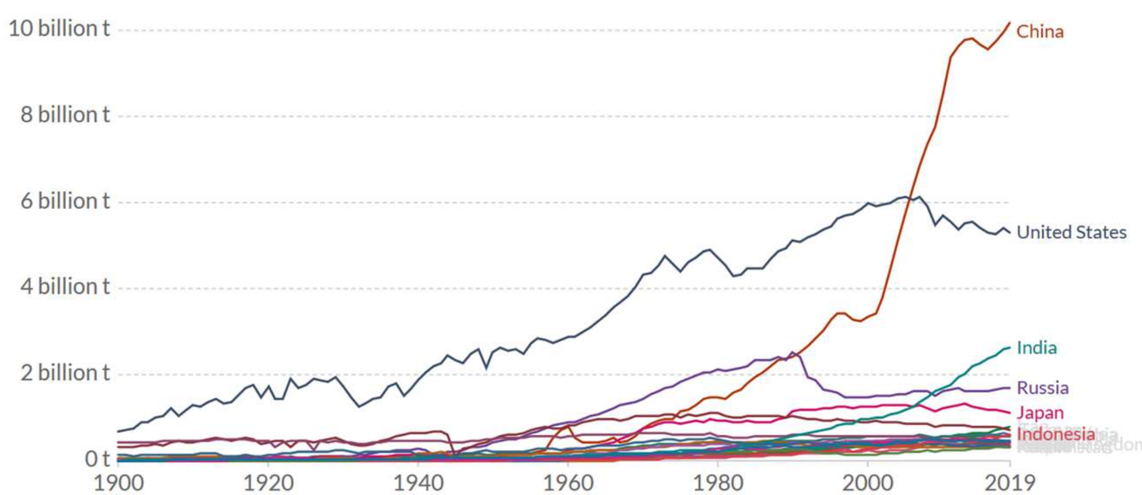
Geography: Who Is Doing What?

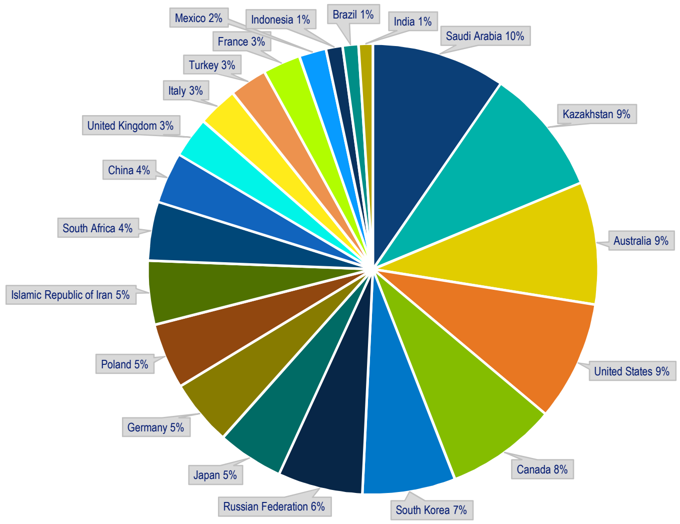
**ENERGY & CEMENT
TOP 20 COUNTRIES**



Source: Global Carbon Project; Carbon Dioxide Information Analysis Centre (CDIAC)
Note: CO_2 emissions are measured on a production basis, meaning they do not correct for emissions embedded in traded goods.
10 OurWorldInData.org/co2-and-other-greenhouse-gas-emissions/ • CC BY

Geography: CO2 Per Capita

FUEL COMBUSTION ONLY
TOP 20 COUNTRIES



Country
Saudi Arabia
Kazakhstan
Australia
United States
Canada
South Korea
Russian Federation
Japan
Germany
Poland
Islamic Republic of Iran
South Africa
China
United Kingdom
Italy
Turkey
France
Mexico
Indonesia
Brazil
India

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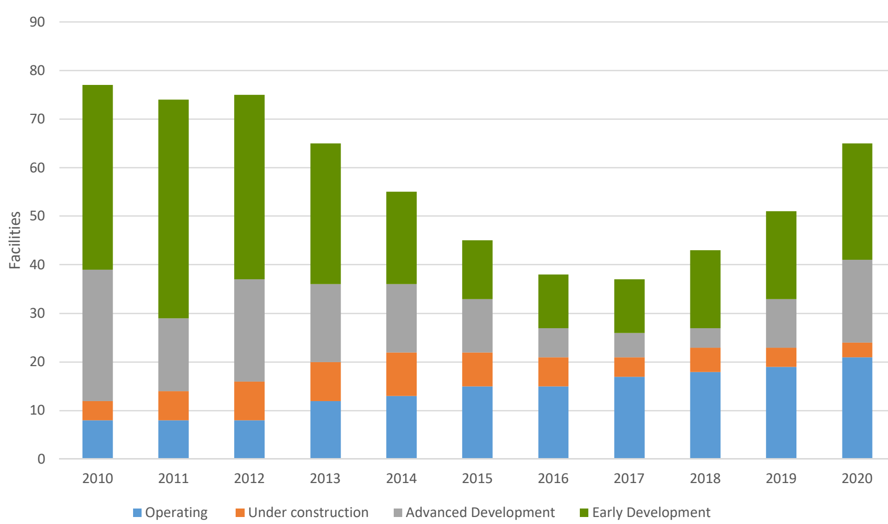
World large-scale CCUS facilities



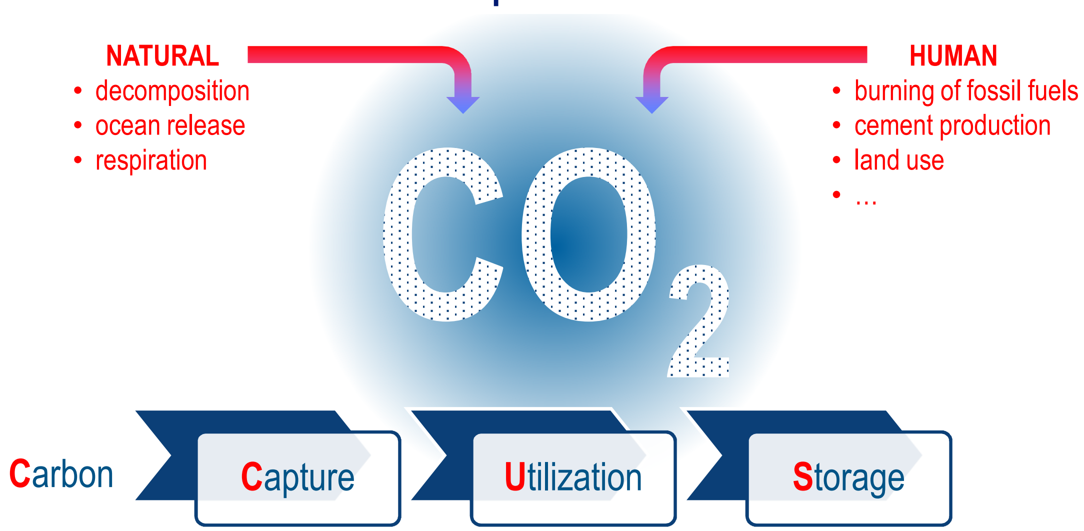
12 Source: IEA

Follow The Money

- The idea that CCUS is “high cost” ignores the bigger picture
- Achieving net-zero goals will be impossible without CCUS
- CCUS cost varies, there is no single number
- CCUS technologies are among the cheapest abatement options
- CCUS supports the integration of renewables in power systems
- CCUS costs are already falling, with potential for further reductions

13 Source: IEA

CCUS or Carbon Sequestration



14

CCUS or Carbon Sequestration

Capture
- Plants
- Industrial objects
- Potentially from air
- …

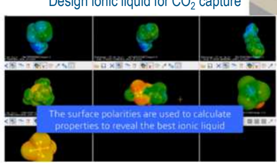
Infrastructure
- Compressors
- Pipelines
- Equipment

Geological Storage
- Saline Acquifer
- Unmineable coal seams
- Depleted oil & gas reservoirs
- …

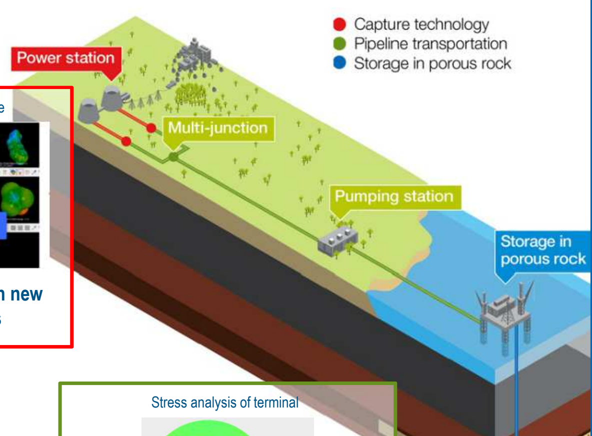
CO_2

Carbon → Capture → Utilization → Storage

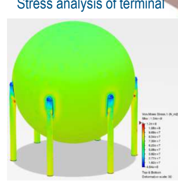
Design ionic liquid for CO_2 capture



Superior CO_2 capture through new fit-for-purpose materials

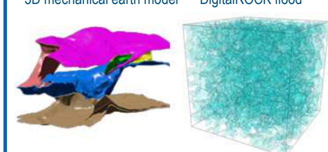


Stress analysis of terminal

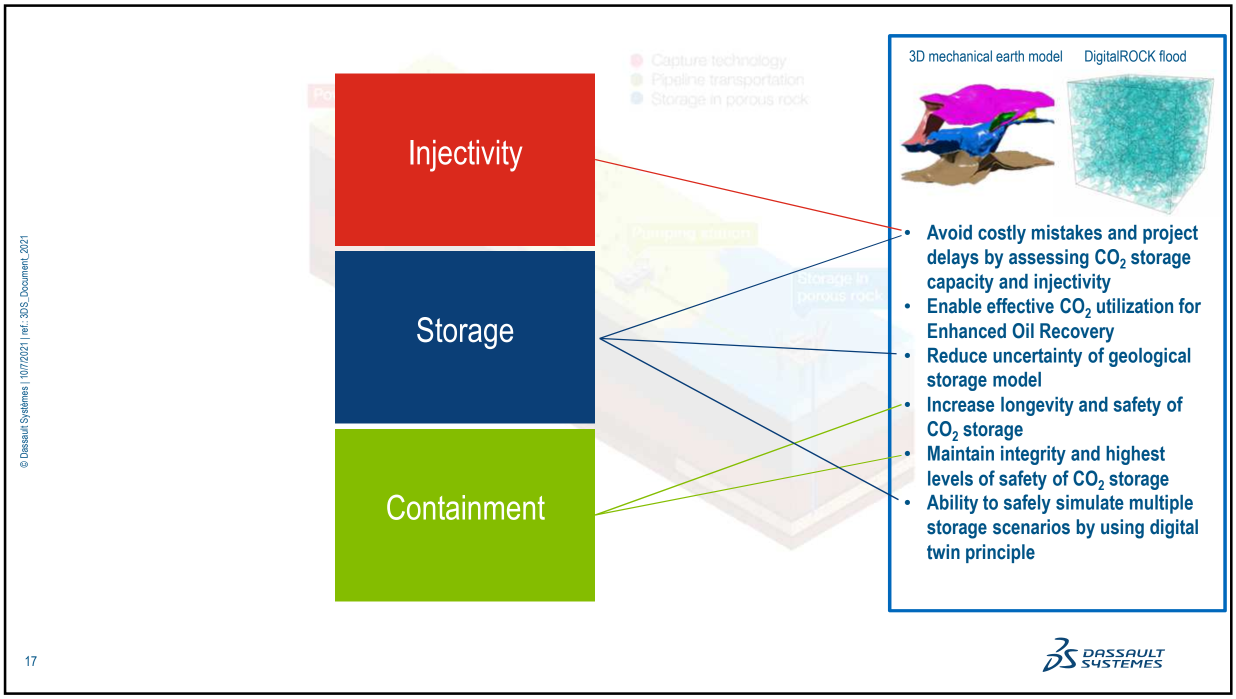


Quick, effective, safe capture and transportation of CO_2

3D mechanical earth model DigitalROCK flood



- **Avoid costly mistakes and project delays by assessing CO_2 storage capacity and injectivity**
- **Enable effective CO_2 utilization for Enhanced Oil Recovery**
- **Reduce uncertainty of geological storage model**
- **Increase longevity and safety of CO_2 storage**
- **Maintain integrity and highest levels of safety of CO_2 storage**
- **Ability to safely simulate multiple storage scenarios by using digital twin principle**



Capture technology
Pipeline transportation
Storage in porous rock
Injectivity
Storage
Containment
3D mechanical earth model
DigitalROCK flood
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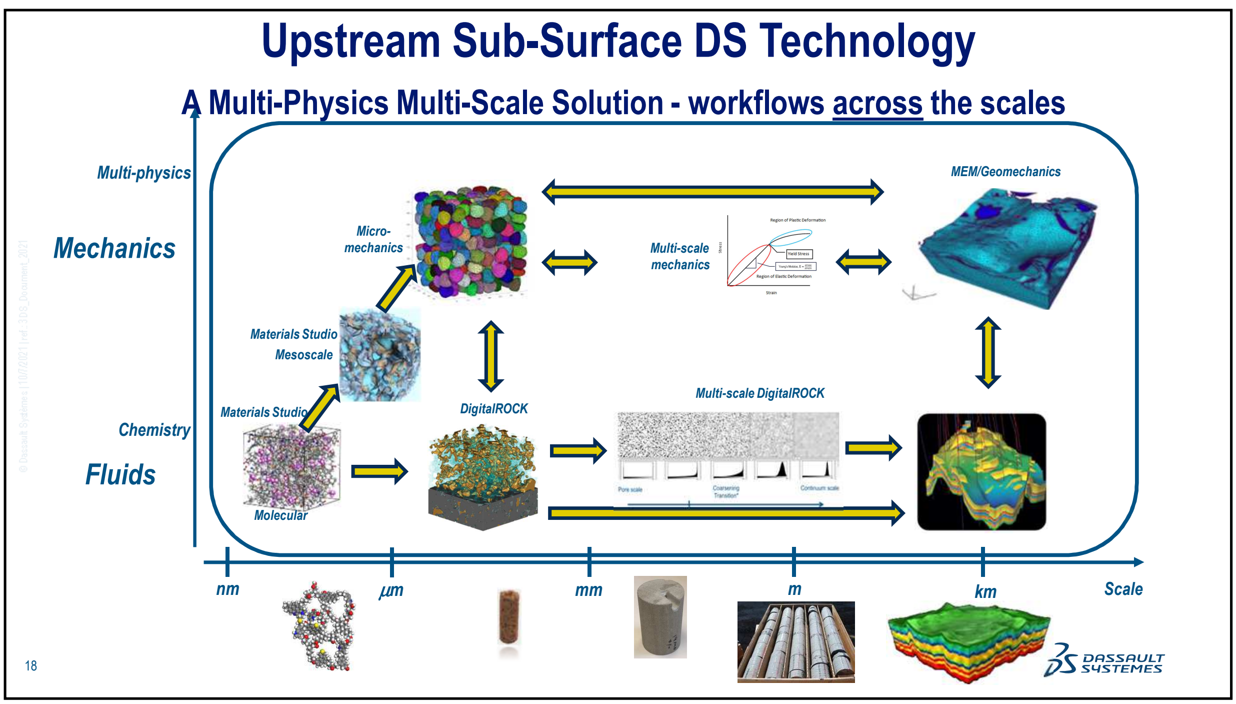

Upstream Sub-Surface DS Technology
A Multi-Physics Multi-Scale Solution - workflows across the scales
Multi-physics
Mechanics
Chemistry
Fluids
Micro-mechanics
Multi-scale mechanics
MEM/Geomechanics
Materials Studio Mesoscale
Materials Studio
Molecular
DigitalROCK
Multi-scale DigitalROCK
nm
µm
mm
m
km
Scale
18
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Our company

A purpose-driven company
Combining Art, Science & Technology
for a more sustainable world

20,000 passionate people
140 nationalities
195 sites
One global R&D / 69 labs

Long-term driven
Majority shareholder control
Revenue: €4,056 millions*
Operating margin: 32%*
*Figures as of FY 2019 / Non-IFRS

12,600 partners
Software, Technology & Architecture
Content & Online services
Sales
Consulting & System Integrators (C&SI)
Education
Research

270,000 customers
11 industries in 140 countries
25 million users
Game-changing
3DEXPERIENCE platform

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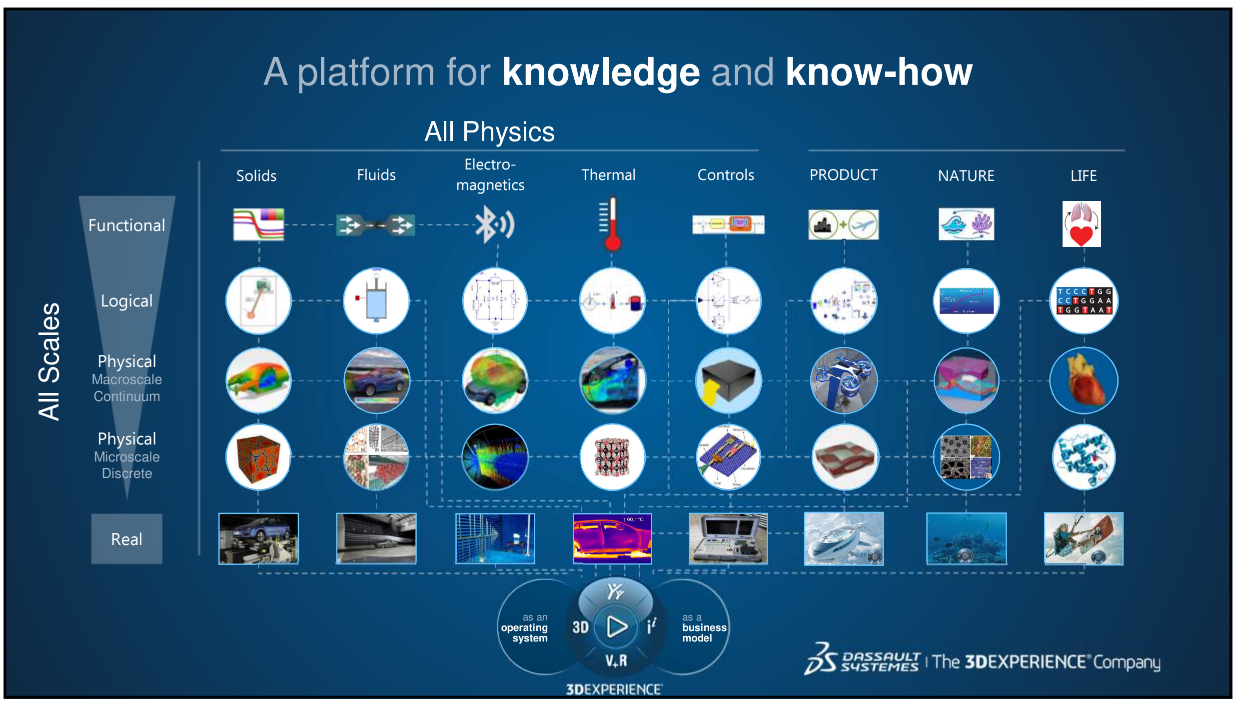
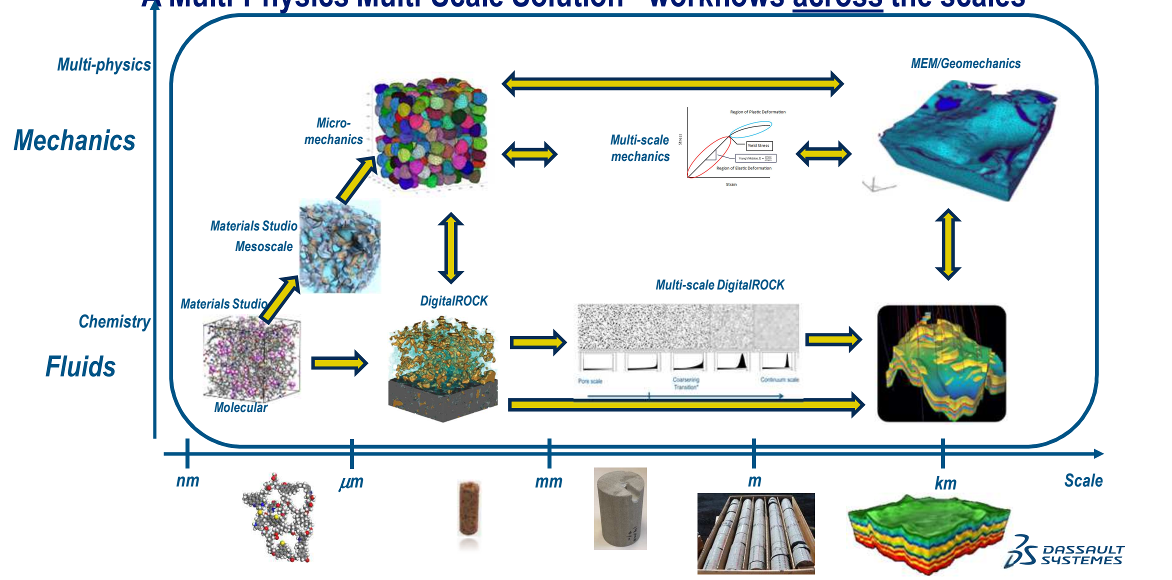


Upstream Sub-Surface DS Technology

A Multi-Physics Multi-Scale Solution - workflows across the scales



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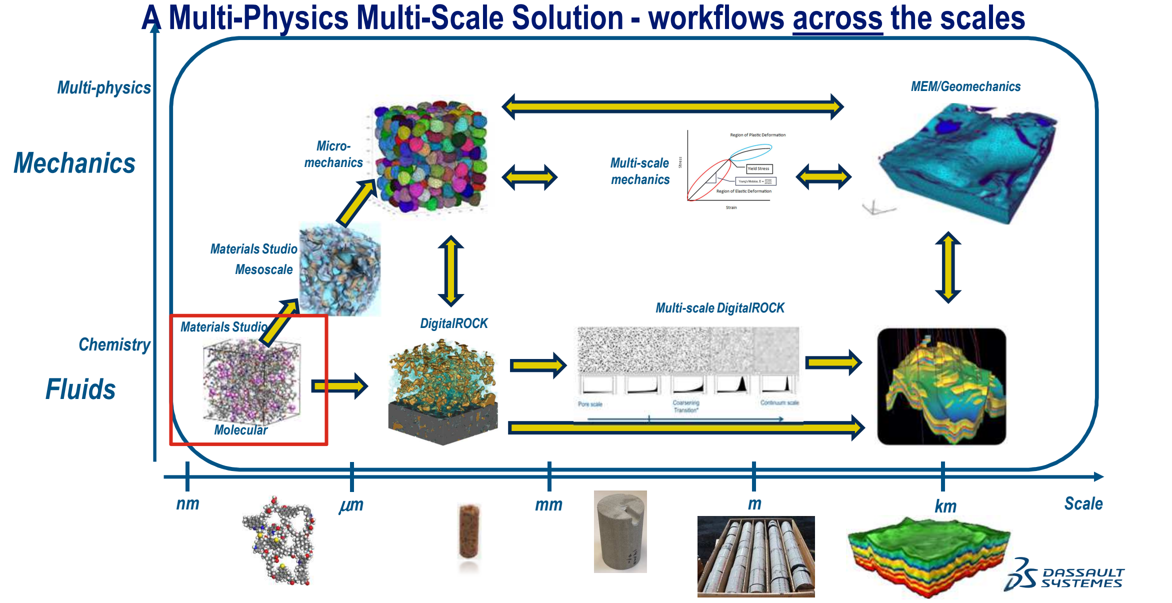
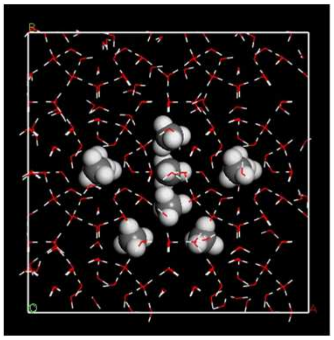


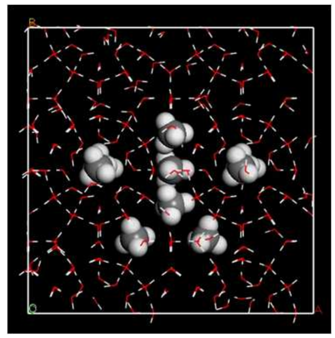
22

Molecular Scale Simulation

Pressure 1



Pressure 2



Dissociation simulations - hydrate formation over time

Ref: Contract Research - Skinner, Subramanian

Upstream Sub-Surface DS Technology

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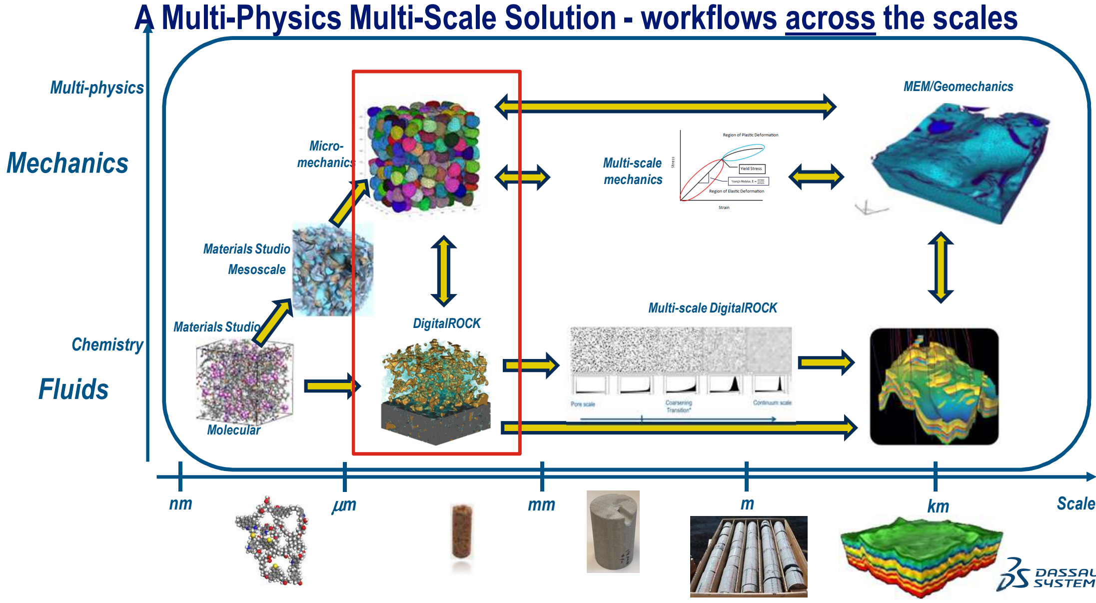

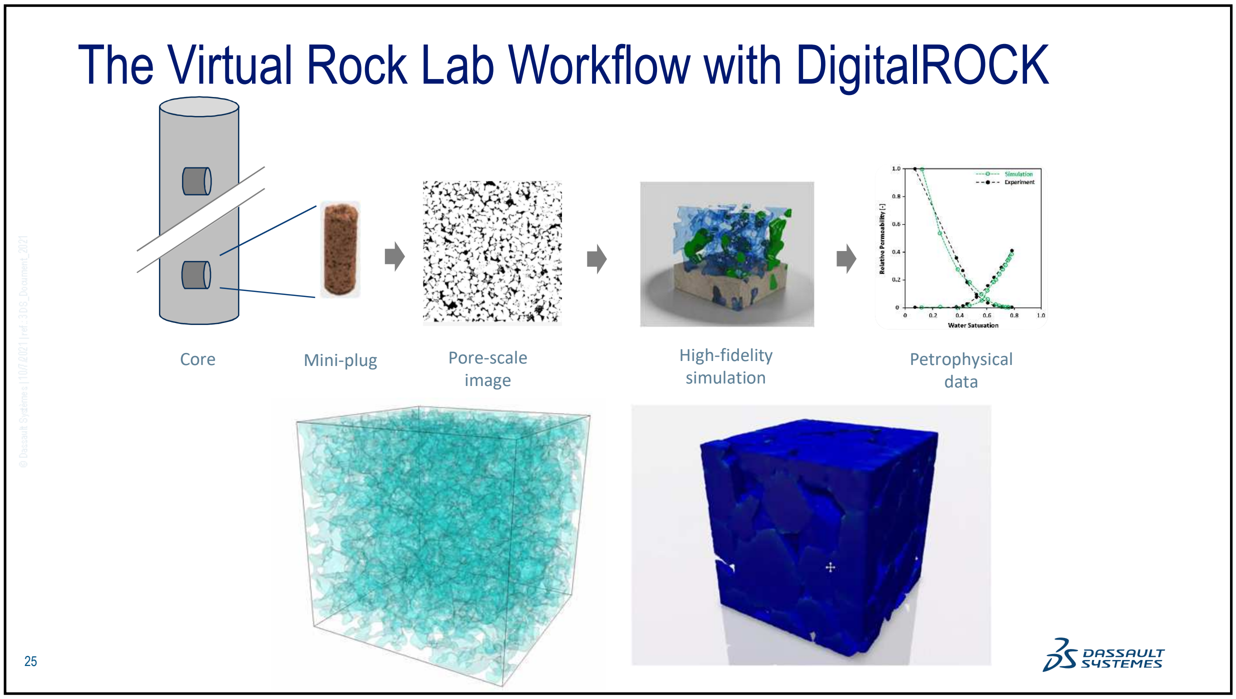
The Virtual Rock Lab Workflow with DigitalROCK
Core
Mini-plug
Pore-scale image
High-fidelity simulation
Petrophysical data
Simulation
Experiment
Relative Permeability [-]
Water Saturation
25
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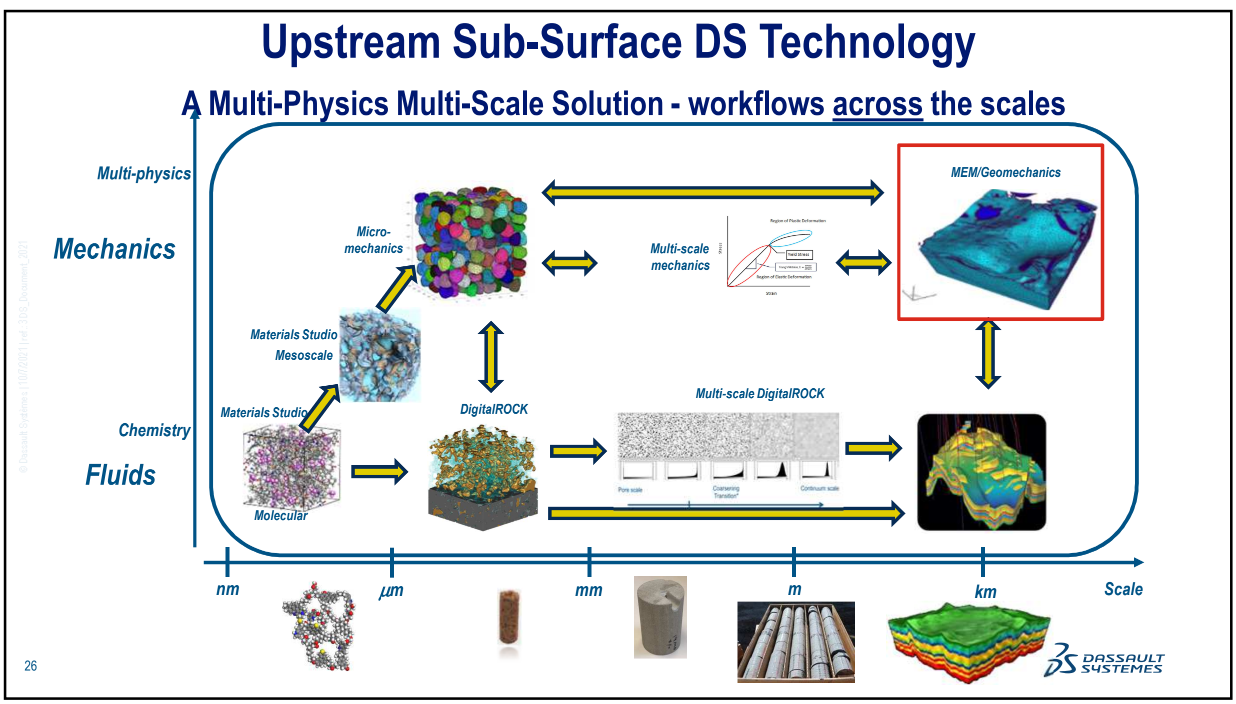
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nm
µm
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Scale
26
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Geomechanics Simulation

27

Geomechanics allows to obtain the stress and strain field of the CO_2 storage formation

Upstream Sub-Surface DS Technology

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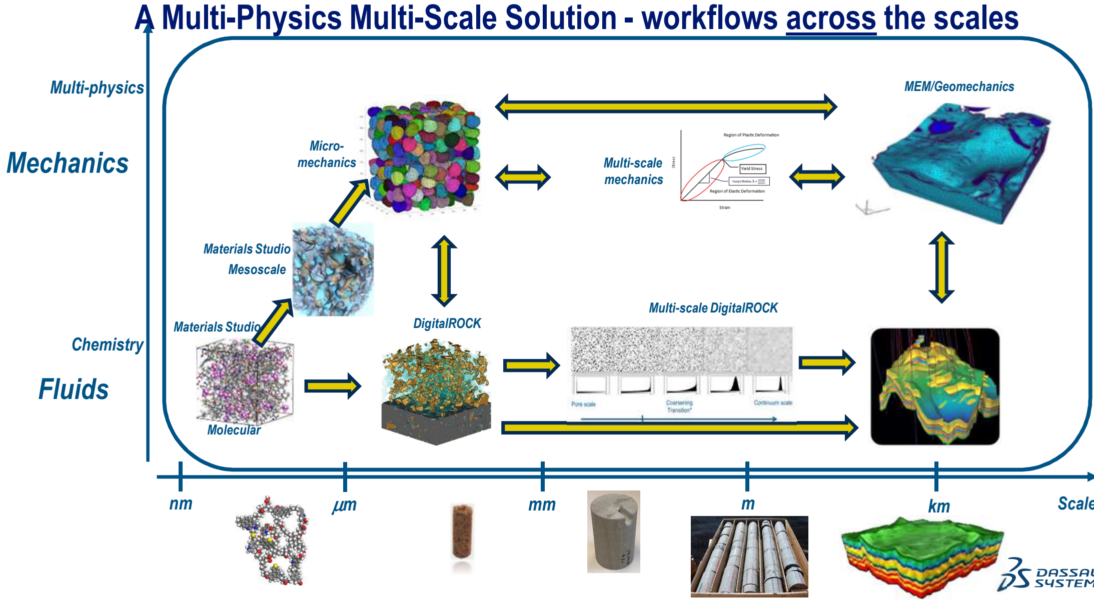

28


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Materials Studio Mesoscale
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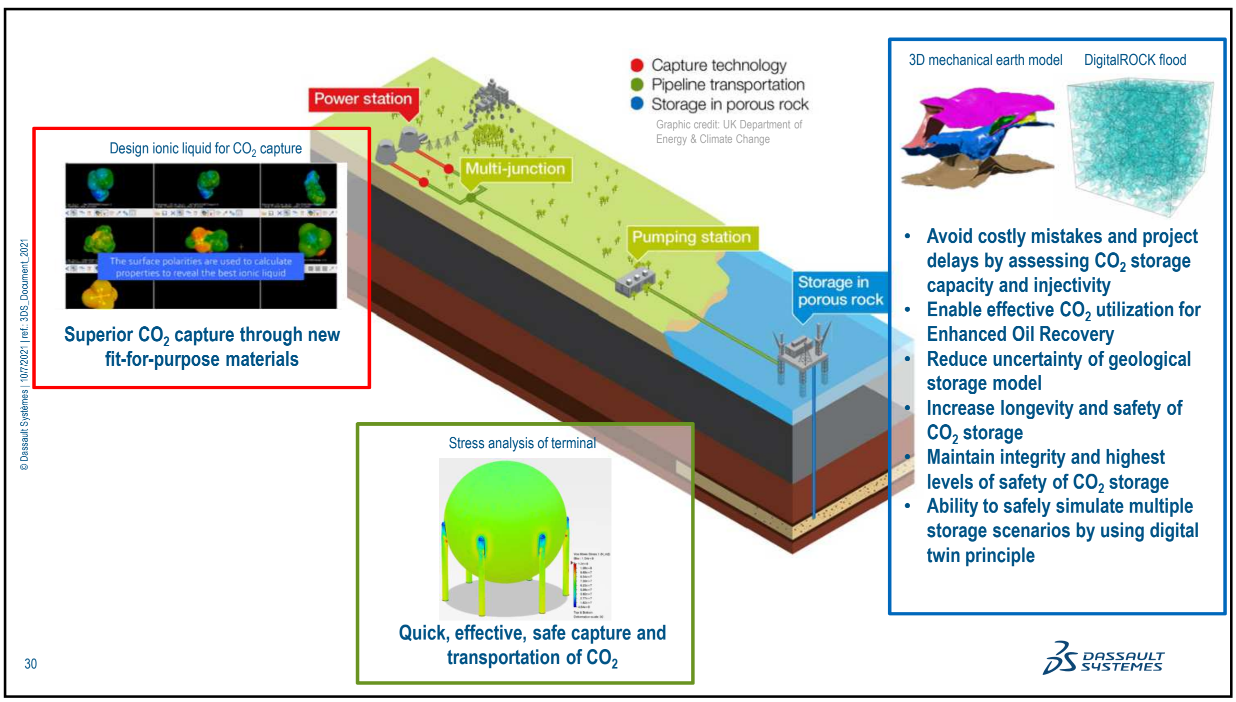
Molecular
DigitalROCK
Multi-scale DigitalROCK
nm
µm
mm
m
km
Scale
Proven
Out of the box


Power station
Capture technology
Pipeline transportation
Storage in porous rock
Graphic credit: UK Department of Energy & Climate Change
Multi-junction
Pumping station
Storage in porous rock
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The surface polarities are used to calculate properties to reveal the best ionic liquid
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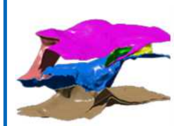
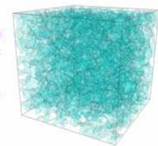
30

Injectivity

Storage

Containment





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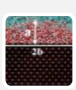
Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

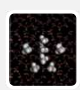
Multiscale Modeling of CO_2 **Storage** for Fluid/Rock Screening

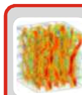

Determination of wettability, interfacial tension and solubility for subsurface fluids (e.g. CO2/Brine or supercritical CO2/Brine) and rock. Informs pore scale digital rock model and other larger scale models used for injectivity and storage assessments.

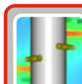

Multiphase pore-scale digital rock floods which capture hysteresis behavior and the impact of varying wettability and interfacial tension. Provides relative permeability (Kr) and capillary pressure (Pc) data for storage (capillary trapping) and injectivity assessments.

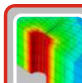

Multiphase multiscale digital rock floods which capture core-scale rock volumes. Provides upscaling of pore-scale Kr and Pc data used for capillary trapping and injectivity assessments (e.g. digital core plug simulations).

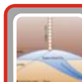
Multiscale/Multiphysics **Injectivity** Assessment


PVT (phase behavior) for impure subsurface fluids, including phase diagrams for hydrates, salts and other solid phases. Informs chemical trapping assessments and injectivity loss assessments.


Pore scale DigitalROCK micromechanics - Provides in-situ pore-space conditions for flow based digital rock analyses (e.g. stress sensitivity).


Perforation tunnel flow analysis on exact perforation tunnel geometries. Provides tunnel injectivity/productivity ratios which incorporate the impact of damage zones and tunnel debris.

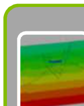

Near well bore injectivity analysis with pressure, temperature and stress fully coupled.


Field scale injectivity analysis with pressure, temperature and stress fully coupled to assess injectivity trends such as gradual loss of injectivity.

Containment Assessment

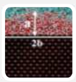

Pore scale DigitalROCK micromechanics - provides effective moduli for larger scale geomechanics analyses.


Fault reactivation assessment with FEA mechanical earth model to assess risk of induced seismicity and leakage through faults.


Caprock integrity assessment with FEA mechanical earth model to assess risk of loss of containment by caprock failure.

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Multiscale Modeling of CO_2 **Storage** for Fluid/Rock Screening



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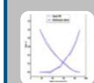

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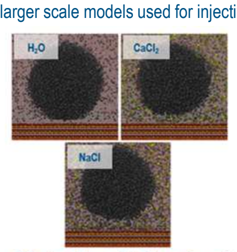
Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Carbon Capture **Utilization and Storage**

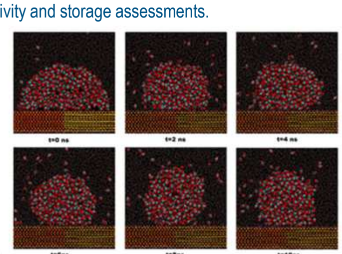
Injectivity | storage

▷ Determination of wettability, interfacial tension and solubility for subsurface fluids (e.g. CO2/Brine or supercritical CO2/Brine) and rock. Informs pore scale digital rock model and other larger scale models used for injectivity and storage assessments.

- **Why?**
  - Interfacial tension and wetting behavior determines CO_2 storage capacity and additionally influences relative flows of CO_2 and brine during injection
  - Better consistency of wetting trends from simulations than what can sometimes be determined experimentally
- **What and How?**
  - Molecular dynamics simulations to model wettability properties
- **Benefit**
  - Improved understanding of molecular interactions between multiphase fluids and mineral phases can be used as inputs to develop larger scale models for surface wetting and determination of fate of CO_2 in reservoirs

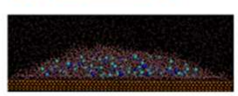


CO_2 droplet on gibbsite surface of kaolinite in presence of water (or brine) with dissolved CO_2



Dewetting process for a CO_2 droplet on silica in an aqueous solution. Detachment distances vary with pure water > 3 M NaCl (1 M $CaCl_2$) > 3 M $CaCl_2$

Ref: Contract Research – Skinner, Schweizer, Subramanian



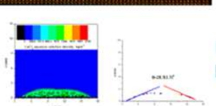


Illustration of contact angle prediction

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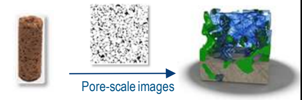
Molecular and meso scale
Pore and grain scale
Core and near well bore scale
Field scale

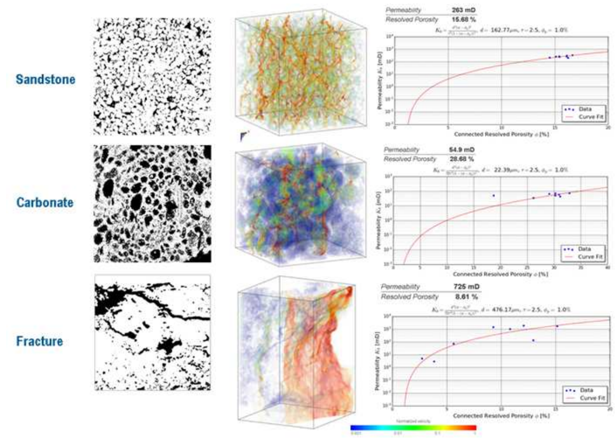
Carbon Capture **Utilization and Storage**



Injectivity storage

▷ Porosity and permeability analysis on digital rock models. Provides input for storage and injectivity assessments.

- **Why**
  - ▷ Suitable subsurface formations should be sufficiently permeable (k) to allow high flow rates without requiring overly high pressure, and have sufficient porosity (Φ) for large volume storage
- **What and how**
  - ▷ Numerical measurements of pore space analysis by SIMULIA DigitalROCK
  - ▷ Evaluate porosity-permeability trend; perform multi-directional analysis to evaluate anisotropy
- **Benefit**
  - ▷ Rich experiences with various rock types
  - ▷ Accurately simulate and extensively validated with oil and gas industry leaders
  - ▷ Powered by best-in-class Lattice-Boltzmann physics



$Injectivity = f(k)$
where k is permeability of rock

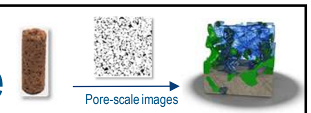
$Storage\ capacity = f(\emptyset)$
where ∅ is porosity of rock

Bachu, S., Bonijoly, D., Bradshaw, J., Burruss, R., Holloway, S., Christensen, N.P., Mathiassen, O.M., 2007. CO2 storage capacity estimation: methodology and gaps. International Journal of Greenhouse Gas Control 1, 430–443.

DASSAULT SYSTEMES

Molecular and meso scale
Pore and grain scale
Core and near well bore scale
Field scale

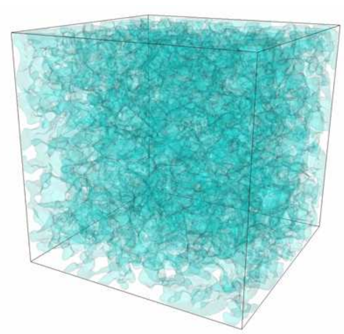
Carbon Capture **Utilization and Storage**

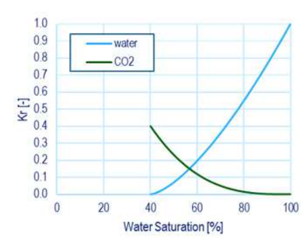


▷ Multiphase pore-scale digital rock floods which capture hysteresis behavior and the impact of varying wettability and interfacial tension. Provides relative permeability (Kr) and capillary pressure (Pc) data for storage (capillary trapping) and injectivity assessments

Injectivity storage

- **Why**
  - ▷ Understanding fundamental relations between relative permeability (kr) and capillary pressure (Pc), saturation, wettability, interfacial tension and pore structure is the basis for reliable prediction of the distribution, displacement of CO_2 and water
- **What and how**
  - ▷ Numerically measurement of kr-Sw and Pc-Sw relations for two-phase flow in reservoir media under wide range of conditions
- **Benefit**
  - ▷ Provide the fastest path from rock to multiphase results by streamlined DigitalROCK workflow
  - ▷ *Accurately simulate and extensively validated with oil and gas industry leaders
  - ▷ Navigate on web-based cloud platform to see computed petrophysical properties and 3d visualizations





*Jerauld, G.R., Fredrich, J., Lane, N., Sheng, Q., Crouse, B., Freed, D.M., Fager, A. and Xu, R., 2017, November. Validation of a workflow for digitally measuring relative permeability. In Abu Dhabi International Petroleum Exhibition & Conference. Society of Petroleum Engineers.

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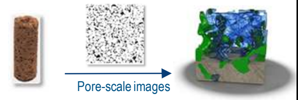

Injectivity | storage

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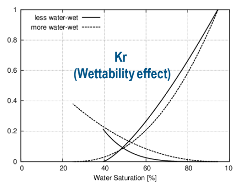

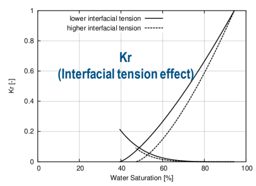

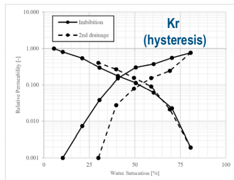

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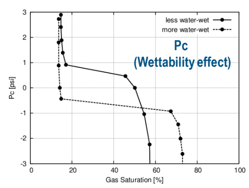

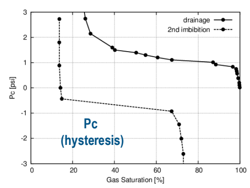

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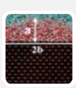
DASSAULT SYSTEMES

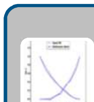
Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Multiscale Modeling of CO_2 **Storage** for Fluid/Rock Screening



Determination of wettability, interfacial tension and solubility for subsurface fluids (e.g. CO2/Brine or supercritical CO2/Brine) and rock. Informs pore scale digital rock model and other larger scale models used for injectivity and storage assessments.

Multiphase pore-scale digital rock floods which capture hysteresis behavior and the impact of varying wettability and interfacial tension. Provides relative permeability (Kr) and capillary pressure (Pc) data for storage (capillary trapping) and injectivity assessments.



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Multiscale/Multiphysics **Injectivity** Assessment

PVT (phase behavior) for impure subsurface fluids, including phase diagrams for hydrates, salts and other solid phases. Informs chemical trapping assessments and injectivity loss assessments.

Pore scale DigitalROCK micromechanics - Provides in-situ pore-space conditions for flow based digital rock analyses (e.g. stress sensitivity).

Perforation tunnel flow analysis on exact perforation tunnel geometries. Provides tunnel injectivity/productivity ratios which incorporate the impact of damage zones and tunnel debris.

Near well bore injectivity analysis with pressure, temperature and stress fully coupled

Field scale injectivity analysis with pressure, temperature and stress fully coupled to assess injectivity trends such as gradual loss of injectivity.

Containment Assessment

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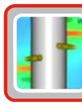

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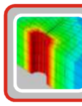

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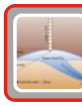

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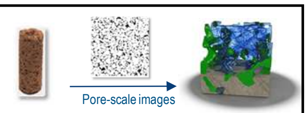
Carbon Capture **Utilization and Storage**



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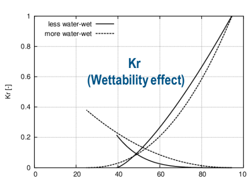
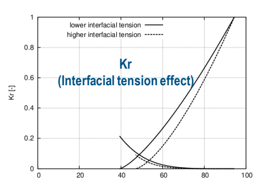
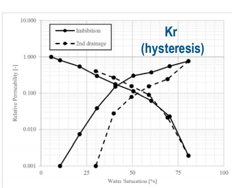
Injectivity | storage







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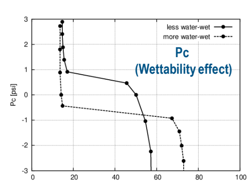

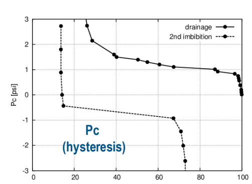

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DASSAULT SYSTEMES

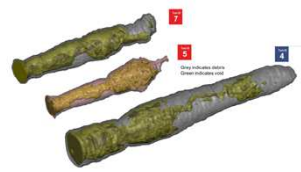
Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

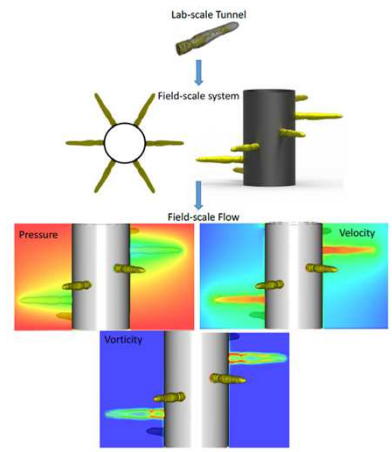
Carbon Capture **Utilization and Storage**

▷ Perforation tunnel flow analysis on exact perforation tunnel geometries. Provides tunnel injectivity/productivity ratios which incorporate the impact of damage zones and tunnel debris.

Injectivity

- **Why**
  - ▷ Perforating can alter formation permeability around perforation tunnels and significantly impact injection/production.
  - ▷ Standard numerical models are based on many assumptions involving tunnel geometry and clean-up, debris and damage characteristics..
- **What and how**
  - ▷ The model leverages the perforation flow laboratory, micro-CT and conventional CT imaging, and advanced simulation approach.
  - ▷ Full-scale three-dimensional flow model accounts for realistic aspects of tunnel geometry, perforation damage and debris that impede the flow.
- **Benefit**
  - ▷ Flow visualization includes fluid velocities, streamlines, pressure gradients, flow rates and corresponding injectivity/productivity.
  - ▷ Provide a realistic prediction of downhole injectivity/productivity as well as evaluable the effects of clean-up techniques.





Advanced Analysis of Clean-up and Productivity from Perforated Rocks Using Computational Fluid Dynamics, SPE-190113-MS, Rajani Satti, Stephen Zuklic, Derek Bale, Baker Hughes, a GE Company, Nils Koliha, Andrew Fager, Gana Balasubramanian, Bernd Crouse, David Freed, Exa Corporation

DASSAULT SYSTEMES

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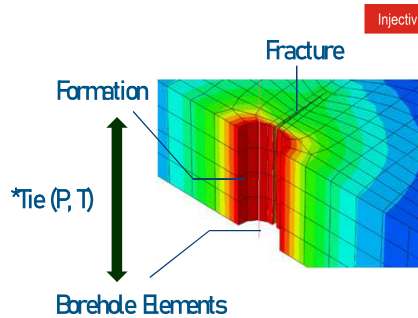
Carbon Capture **Utilization and Storage**

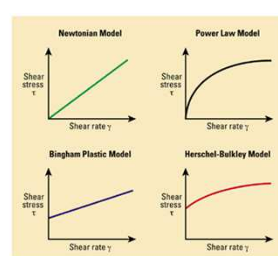
▷ Near well bore injectivity analysis with pressure, temperature and stress fully coupled.

Injectivity

ABAQUS offers a broad range of capabilities for end-to-end modeling of geothermal processes.

- Fluid Transport in Borehole– Specially formulated fluid pipe and connector elements
  - FP2D2 (in 2D without Temp.), FP3D2 (in 3D without Temp.)
  - FP2D2T (in 2D with Temp.), FP3D2T (in 3D Temp.)
  - Full family of built-in pipe/connector loss terms
- Borehole-Formation Coupling – Pressure and temperature transmission between the formation and the borehole through *TIE functionality.
- Formation Behavior – Fully coupled thermal-hydro-mechanical formulation.
  - Deformation: Linear and non-linear elasticity models.
  - Failure: Ductile failure (plasticity) ; Brittle failure: fracture (CZM, XFEM)
- Fluid Rheology – Fluid Supports a variety of fluid rheology behaviors e.g. Newtonian, Power Law, Bingham Plastic, Herschel-Bulkley.





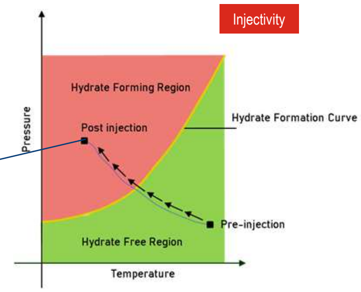
SAULT
EMES

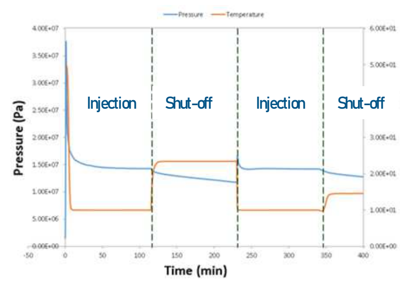
Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Carbon Capture **Utilization and Storage**

▷ Near well bore injectivity analysis with pressure, temperature and stress fully coupled.

- **Why**
  - Common cause of sudden loss of injectivity: Hydrate formation (detrimental to downhole and surface facilities)
  - Hydrates are solid phases that form when gas mix with water at low temperatures and high pressures
- **What and how**
  - Coupled thermal-hydro-mechanical numerical simulation
  - Temperature rises back while pressure declines. The hydrates become thermodynamically unstable ("melt away")
- **Benefit**
  - Simulations can help us design an intermittent injection process – alternating between "injection" and "Shut-offs"





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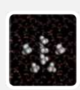
Multiscale/Multiphysics **Injectivity** Assessment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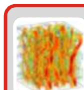
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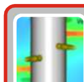
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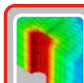
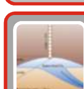

Near well bore injectivity analysis with pressure, temperature and stress fully coupled.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DASSAULT SYSTEMES

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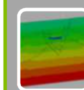


Caprock integrity assessment with FEA mechanical earth model to assess risk of loss of containment by caprock failure.

DASSAULT SYSTEMES

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Carbon Capture **Utilization and Storage**

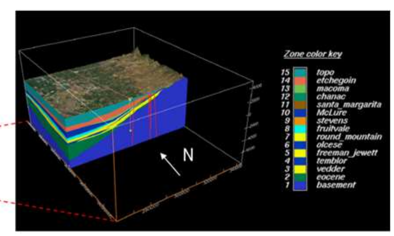
▷ Fault reactivation assessment with FEA mechanical earth model to assess risk of induced seismicity and leakage through faults.

containment

- Why
  - Fault reactivation can possibly compromise fault sealing capacity or induce seismic events
- What and how
  - Perform a geomechanical analysis for an industry-scale carbon sequestration project located in the southern San Joaquin Basin, California USA
- Benefit
  - Advanced geomechanics and parallel computing capabilities
  - Simulation results show a reactivation of the faults with a limited moment magnitude
  - Moment magnitude is an output related to fault slippage and rupture area

Range of southern San Joaquin Basin regional model

Geologic model (Wagoner, 2009)



Moment magnitude
magnitude scale of seismic event

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Carbon Capture **Utilization and Storage**

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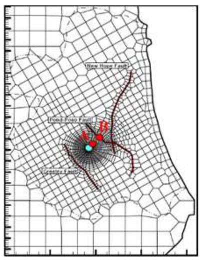
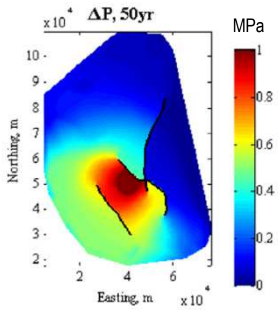
containment

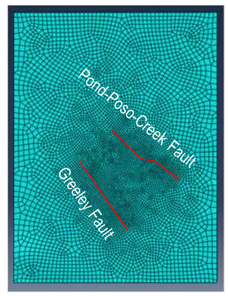
Reservoir simulation grid



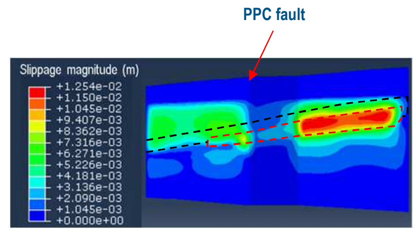
Pressure buildup



Finite element mesh



Distribution of fault slippage



- Inject 5 Mt CO_2 per for 50 years
- Sealing faults are assumed based on field observation
- A Coulomb friction model is used to represent fault slip behaviour

DASSAULT SYSTEMES

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Carbon Capture **Utilization and Storage**

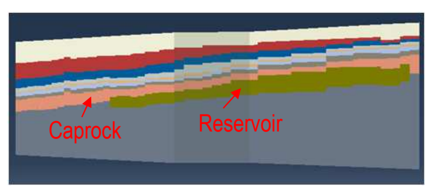
▷ Caprock integrity assessment with FEA mechanical earth model to assess risk of loss of containment by caprock failure.

containment

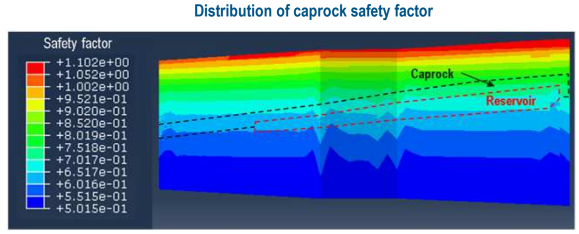
- Why
  - ▷ Caprock has a very low permeability and acts as a vertical flow barrier. It is critical for longevity and safety of CO_2 storage
- What and how
  - ▷ Perform a finite element geomechanical simulation to analyze the stress and strain behavior within the caprock
- Benefit
  - ▷ Simulation results include safe factor based on Mohr-Coulomb criterion or cumulative plastic deformation
  - ▷ These results are then used to assess the likelihood of fracture slip, which may comprise the caprock seal integrity

Safety factor based on Mohr-Coulomb criterion

Geologic cross section



Distribution of caprock safety factor



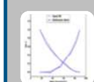
DASSAULT SYSTEMES

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Multiscale Modeling of CO_2 **Storage** for Fluid/Rock Screening

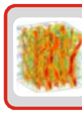

Determination of wettability, interfacial tension and solubility for subsurface fluids (e.g. CO2/Brine or supercritical CO2/Brine) and rock. Informs pore scale digital rock model and other larger scale models used for injectivity and storage assessments.

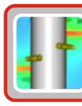

Multiphase pore-scale digital rock floods which capture hysteresis behavior and the impact of varying wettability and interfacial tension. Provides relative permeability (Kr) and capillary pressure (Pc) data for storage (capillary trapping) and injectivity assessments.

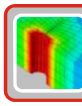

Multiphase multiscale digital rock floods which capture core-scale rock volumes. Provides upscaling of pore-scale Kr and Pc data used for capillary trapping and injectivity assessments (e.g. digital core plug simulations).

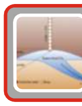
Multiscale/Multiphysics **Injectivity** Assessment


PVT (phase behavior) for impure subsurface fluids, including phase diagrams for hydrates, salts and other solid phases. Informs chemical trapping assessments and injectivity loss assessments.


Pore scale DigitalROCK micromechanics - Provides in-situ pore-space conditions for flow based digital rock analyses (e.g. stress sensitivity).


Perforation tunnel flow analysis on exact perforation tunnel geometries. Provides tunnel injectivity/productivity ratios which incorporate the impact of damage zones and tunnel debris.

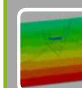

Near well bore injectivity analysis with pressure, temperature and stress fully coupled.


Field scale injectivity analysis with pressure, temperature and stress fully coupled to assess injectivity trends such as gradual loss of injectivity.

Containment Assessment


Pore scale DigitalROCK micromechanics - provides effective moduli for larger scale geomechanics analyses.


Fault reactivation assessment with FEA mechanical earth model to assess risk of induced seismicity and leakage through faults.


Caprock integrity assessment with FEA mechanical earth model to assess risk of loss of containment by caprock failure.

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Contact us

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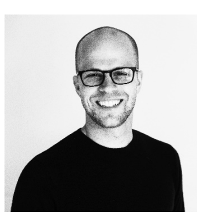

Andrew Fager
Senior Manager, Energy Industry Processes
andrew.fager@3ds.com

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51

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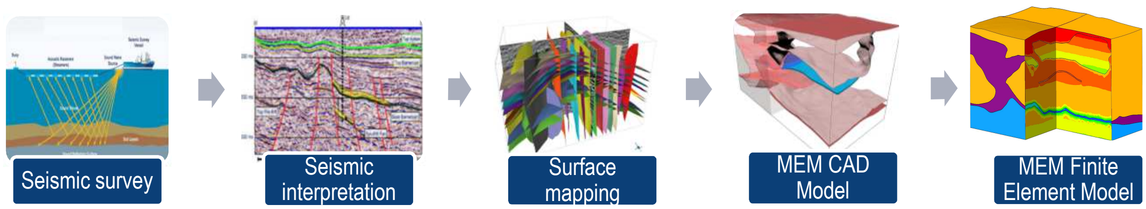
52

Geomechanics Simulation



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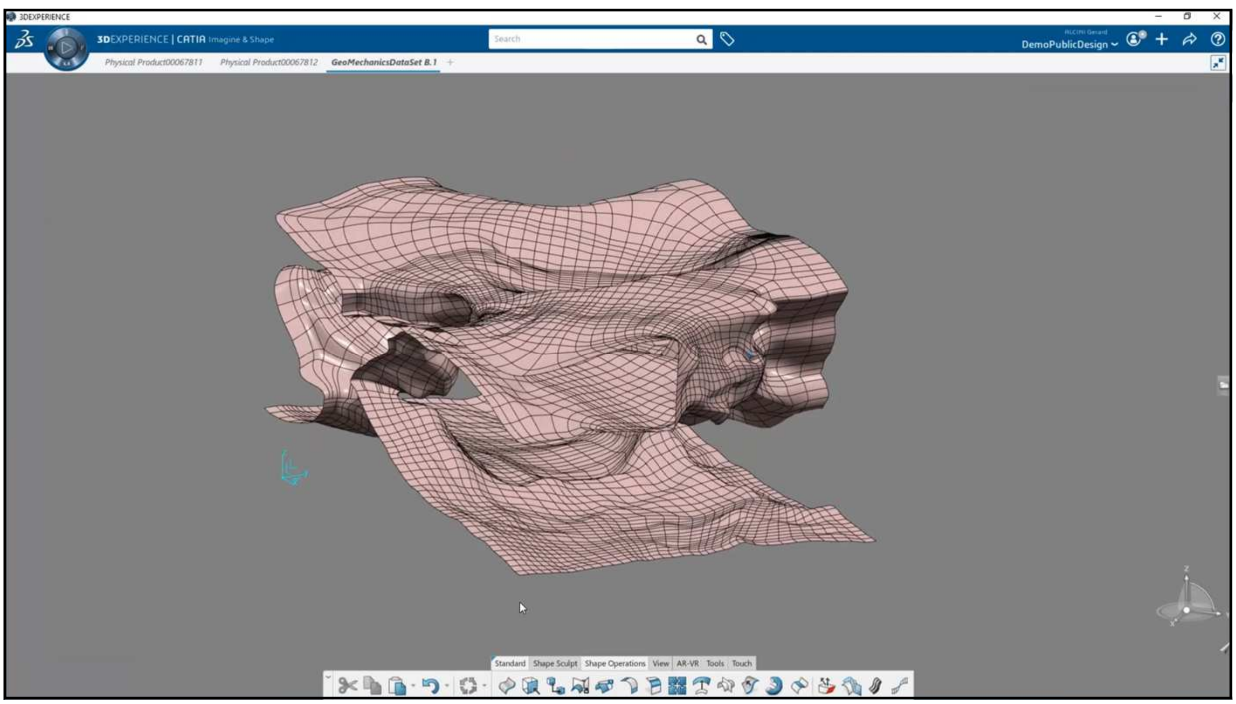


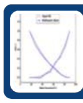
Project 1: Multiscale Modeling of CO_2 Plume for Fluid/Rock Screening

Mineralogy Dependent Wettability (Molecular Dynamics) - deliverable: 6x contact angles
- 3x fluid pairs (supercritical CO2/Brine at 3x Pressure/Temperature/Brine conditions)
- 2x rock surfaces (e.g. clay and quartz)

Molecular Dynamics IFT - deliverable: 3x IFT values
- 3x fluid pairs (supercritical CO2/Brine at 3x Pressure/Temperature/Brine conditions)

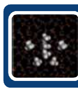
Molecular Dynamics Solubility - deliverable: 3x solubility results
- 3x fluid pairs (supercritical CO2/Brine at 3x Pressure/Temperature/Brine conditions)

Pore scale DigitalROCK Relative permeability - deliverable: 12x pore scale Kr curves
- 6x MicroCTs
- 2x Kr/MicroCT (drainage + imbibition)

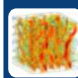


Plug scale DigitalROCK Relative permeability - deliverable: 6x plug scale Kr curves
- 3x MacroCTs
- 2x Kr/MacroCT (drainage + imbibition)

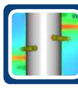
Project 2: Multiscale/Multiphysics Injectivity Assessment



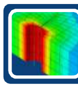
PVT (phase behavior) for impure subsurface fluids, including phase diagrams for hydrates, salts and other solid phases - deliverable: 1x PVT result



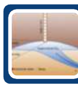
Pore scale DigitalROCK micromechanics - deliverable: 3x pore scale stress-dependent permeability, 3x pore scale stress-dependent porosity, 6x pore scale stress-dependent relative permeability
- 3x MicroCTs
- 1x stress-dependent porosity, stress-dependent permeability/MicroCT
- 2x stress-dependent relative permeability/MicroCT (drainage + imbibition)



Perforation tunnel flow analysis on scanned perforation tunnel geometries - deliverable: injectivity ratio for 3x perforation tunnels



Near well bore injectivity analysis with pressure, temperature and stress fully coupled - deliverable: 3x near well bore injection programs, 1x near well bore Abaqus model

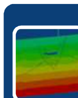


Field scale injectivity analysis with pressure, temperature and stress fully coupled - deliverable: 3x field scale injectivity scenarios, 1x field scale Abaqus model

Project 3: Containment Assessment

Pore scale DigitalROCK micromechanics - deliverable: 3x elastic modulus
- 3x MicroCTs
- 1x elastic modulus/MicroCT

Fault reactivation assessment with FEM mechanical earth model - deliverable: 3x moment magnitude of a seismic event corresponding to 3x injection scenarios, 1x field scale Abaqus model



Caprock integrity assessment with FEM mechanical earth model - deliverable: 3x safety factor distribution within caprock corresponding to 3x injection scenarios, 1x field scale Abaqus model

55

DASSAULT SYSTEMES

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

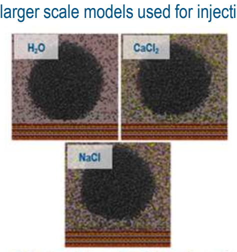
Carbon Capture **Utilization and Storage**

Injectivity | storage | containment

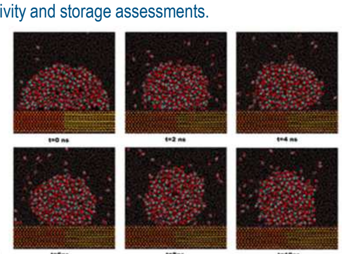
- Determination of wettability, interfacial tension and solubility for subsurface fluids (e.g. CO2/Brine or supercritical CO2/Brine) and rock. Informs pore scale digital rock model and other larger scale models used for injectivity and storage assessments.

Slide 1 of 2

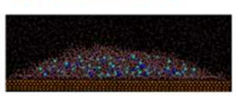
- **Why?**
  - Interfacial tension and wetting behavior determines CO_2 storage capacity and additionally influences relative flows of CO_2 and brine during injection
  - Better consistency of wetting trends from simulations than what can sometimes be determined experimentally
- **What and How?**
  - Molecular dynamics simulations to model wettability properties
- **Benefit**
  - Improved understanding of molecular interactions between multiphase fluids and mineral phases can be used as inputs to develop larger scale models for surface wetting and determination of fate of CO_2 in reservoirs



CO_2 droplet on gibbsite surface of kaolinite in presence of water (or brine) with dissolved CO_2



Dewetting process for a CO_2 droplet on silica in an aqueous solution. Detachment distances vary with pure water > 3 M NaCl (1 M $CaCl_2$) > 3 M $CaCl_2$



Ref: Contract Research – Skinner, Schweizer, Subramanian

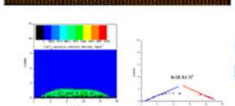


Illustration of contact angle prediction

DASSAULT SYSTEMES

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

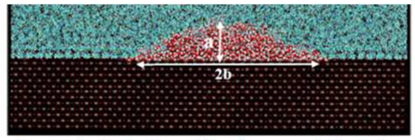
Carbon Capture **Utilization and Storage**

Injectivity | storage | containment

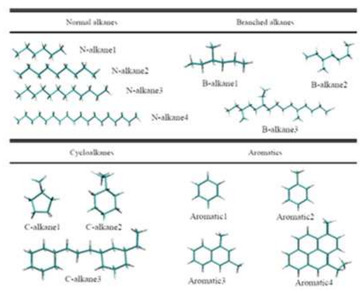
▷ Determination of wettability, interfacial tension and solubility for subsurface fluids (e.g. CO2/Brine or supercritical CO2/Brine) and rock. Informs pore scale digital rock model and other larger scale models used for injectivity and storage assessments.

Slide 2 of 2

- **Why?**
  - ▷ Understand how wettability is altered as a function of changes to brine composition
- **What and How?**
  - ▷ Molecular dynamics to model contact angles, IFT
  - ▷ Surfaces interacting with different oil models and brine compositions will result in varying levels of adhesion between components depending on composition of phases
  - ▷ Polar fraction of 52% in a crude oil-water yields IFT of 24.7 mN/m, in the range of experimentally determined values at same P-T conditions
- **Benefit**
  - ▷ Simulations of complex fluids at experimentally relevant conditions can act as a proxy for difficult to make measurements



Snapshot of water droplet on calcite surface surrounded by oil phase



Sample of oil phase components

Ref: Contract Research – Skinner, Schweizer, Subramanian

DASSAULT SYSTEMES

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

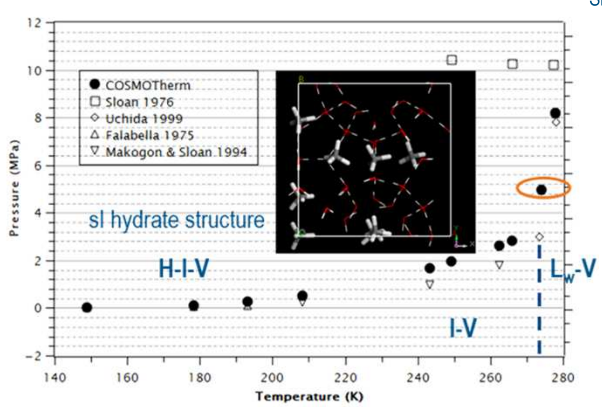
Carbon Capture **Utilization and Storage**

Injectivity | storage | containment

▷ PVT (phase behavior) for impure subsurface fluids, including phase diagrams for hydrates, salts and other solid phases. Informs chemical trapping assessments and injectivity loss assessments.

Slide 1 of 2

- **Why?**
  - ▷ Understand P-T relationships for clathrates, including mixed molecule systems
- **What and How?**
  - ▷ Ab initio molecular simulations based on COSMOTherm, QM or Phase Field to model phase behavior of pure and mixed component systems
- **Benefit**
  - ▷ COSMOTherm data is consistent with data from various experimental sources (shown), some obtained under non-equilibrium conditions
    - Data point near 275 (circled) is super-imposed on another experimental data point
  - ▷ Output part of an effort with The University of Western Australia



H = Hydrate sI, I = Ice, V = Methane Vapor, Lw = Liquid water

Ref: Contract Research – Skinner, Subramanian

DASSAULT SYSTEMES

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Carbon Capture **Utilization and Storage**

Injectivity | storage | containment

▷ PVT (phase behavior) for impure subsurface fluids, including phase diagrams for hydrates, salts and other solid phases. Informs chemical trapping assessments and injectivity loss assessments.

Slide 2 of 2

Dissociation simulations

Movies of sI clathrate hydrate system evolution w.r.t. time

Evolution inline with diffusion coeff. analysis

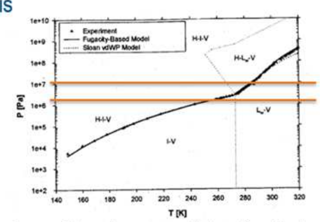
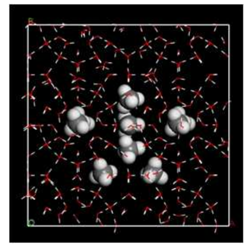


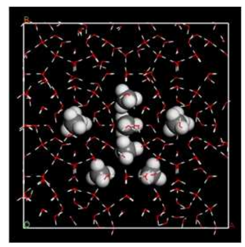
Figure 3.5 Phase diagram of the methane structure I hydrate (from Klauda and Sandler, 2002).
H = Hydrate sI, I = Ice, V = Methane Vapor, Lw = Liquid water.

Ref: Contract Research – Skinner, Subramanian

250 K, 2 MPa



250 K, 10 MPa



DASSAULT SYSTEMES

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Carbon Capture **Utilization and Storage**

Injectivity | storage | containment

▷ Grain compression and compaction analyses on digital rock models with FEA (Abaqus) micromechanics. Provides in-situ pore-space conditions for flow based digital rock analyses (e.g. stress sensitivity) and effective moduli for larger scale geomechanics analyses.

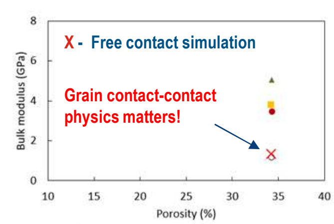
- Why
  - ▷ 3D tomography images are obtained at ambient conditions (no stress effect)
- What and how
  - ▷ Use Abaqus to simulate subsurface pressure conditions
- Benefit
  - ▷ Simulate fluid flow properties under compression effect
  - ▷ Simulate linear elastic response
  - ▷ Grain relocation capability unique in industry

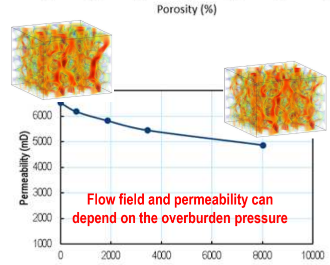
Fontainebleau Sandstone

Stress-dependent permeability

Stress-dependent porosity

Elastic modulus





Prediction of rock elastic moduli based on a micromechanical finite element model. Zhuang Sun, Rafael Salazar-Tio, Luca Duranti, Bernd Crouse, Andrew Fager, Ganapathi Balasubramanian. *Computers and Geotechnics*. 2021

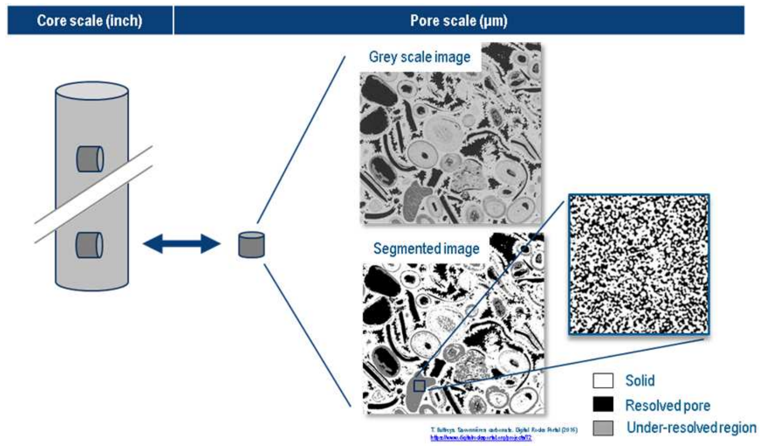
Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Carbon Capture **Utilization and Storage**

Injectivity | storage

- Multiphase multiscale digital rock floods which capture core-scale rock volumes. Provides upscaling of pore-scale Kr and Pc data used for capillary trapping and injectivity assessments (e.g. digital core plug simulations).

- Why
  - There is the trade-off between rock image resolution and representative elemental volume.
  - In carbonate and other heterogeneous multiscale rocks, large scale pore structures are connected by small scale pore structures.
- What and how
  - Couple direct and continuum simulations
  - Use pre-computed fully-resolved physical properties to apply to under-resolved regions
  - Has potential to obtain relative permeability (Kr) and capillary pressure (Pc) data in upscaling towards core-scale with reduced computational expense
- Benefit
  - Work with even a small rock sample; whole core is not required



$Injectivity_{CO_2} \sim kr$ $\quad$ $Storage\ capacity_{CO_2} \sim S_{wi}(kr, Pc)$

DASSAULT SYSTEMES

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

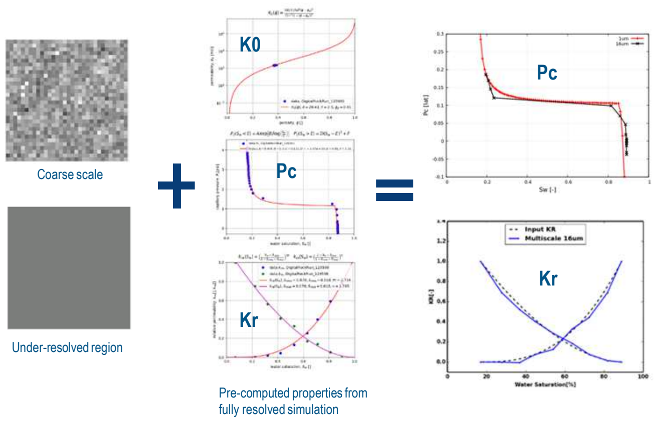
Carbon Capture **Utilization and Storage**

Injectivity | storage

- Multiphase multiscale digital rock floods which capture core-scale rock volumes. Provides upscaling of pore-scale Kr and Pc data used for capillary trapping and injectivity assessments (e.g. digital core plug simulations).

$Injectivity_{CO_2} \sim kr$

$Storage\ capacity_{CO_2} \sim S_{wi}(kr, Pc)$



- Couple direct and continuum simulations
- Use pre-computed fully-resolved physical properties to apply to under-resolved regions
- Has potential to obtain relative permeability (Kr) and capillary pressure (Pc) data in upscaling towards core-scale with reduced computational expense

DASSAULT SYSTEMES

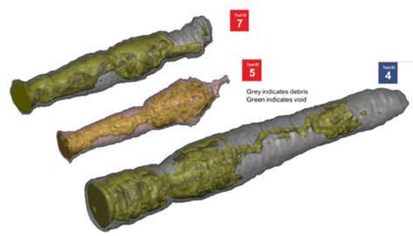
Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

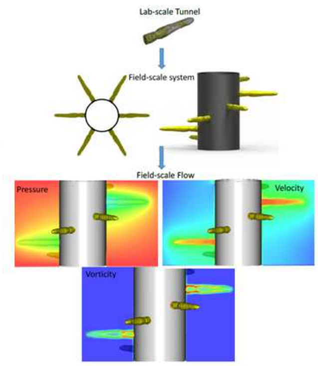
Carbon Capture **Utilization and Storage**

▷ Perforation tunnel flow analysis on exact perforation tunnel geometries. Provides tunnel injectivity/productivity ratios which incorporate the impact of damage zones and tunnel debris.

Injectivity

- **Why**
  - ▷ Perforating can alter formation permeability around perforation tunnels and significantly impact injection/production.
  - ▷ Standard numerical models are based on many assumptions involving tunnel geometry and clean-up, debris and damage characteristics..
- **What and how**
  - ▷ The model leverages the perforation flow laboratory, micro-CT and conventional CT imaging, and advanced simulation approach.
  - ▷ Full-scale three-dimensional flow model accounts for realistic aspects of tunnel geometry, perforation damage and debris that impede the flow.
- **Benefit**
  - ▷ Flow visualization includes fluid velocities, streamlines, pressure gradients, flow rates and corresponding injectivity/productivity.
  - ▷ Provide a realistic prediction of downhole injectivity/productivity as well as evaluable the effects of clean-up techniques.





Advanced Analysis of Clean-up and Productivity from Perforated Rocks Using Computational Fluid Dynamics, SPE-190113-MS, Rajani Satti, Stephen Zuklic, Derek Bale, Baker Hughes, a GE Company, Nils Koliha, Andrew Fager, Gana Balasubramanian, Bernd Crouse, David Freed, Exa Corporation

DASSAULT SYSTEMES

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

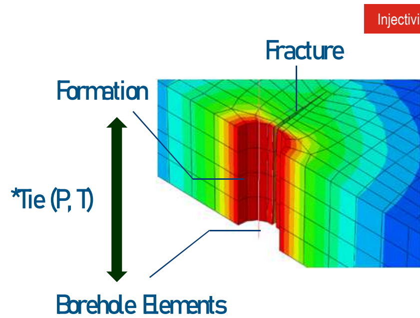
Carbon Capture **Utilization and Storage**

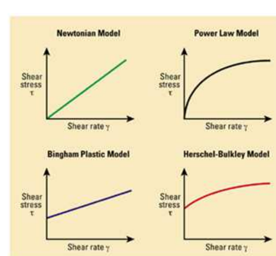
▷ Near well bore injectivity analysis with pressure, temperature and stress fully coupled.

Injectivity

ABAQUS offers a broad range of capabilities for end-to-end modeling of geothermal processes.

- Fluid Transport in Borehole– Specially formulated fluid pipe and connector elements
  - FP2D2 (in 2D without Temp.), FP3D2 (in 3D without Temp.)
  - FP2D2T (in 2D with Temp.), FP3D2T (in 3D Temp.)
  - Full family of built-in pipe/connector loss terms
- Borehole-Formation Coupling – Pressure and temperature transmission between the formation and the borehole through *TIE functionality.
- Formation Behavior – Fully coupled thermal-hydro-mechanical formulation.
  - Deformation: Linear and non-linear elasticity models.
  - Failure: Ductile failure (plasticity) ; Brittle failure: fracture (CZM, XFEM)
- Fluid Rheology – Fluid Supports a variety of fluid rheology behaviors e.g. Newtonian, Power Law, Bingham Plastic, Herschel-Bulkley.





SAULT
EMES

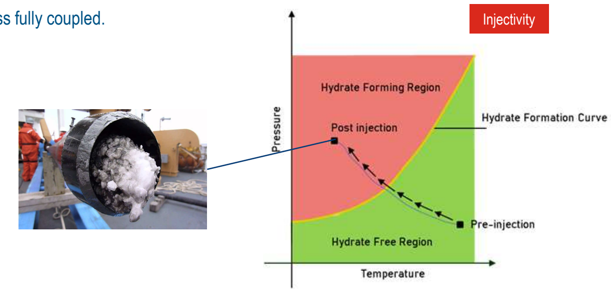
Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

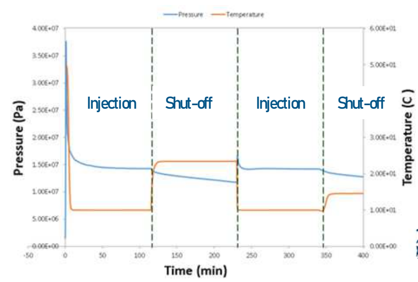
Carbon Capture **Utilization and Storage**

▷ Near well bore injectivity analysis with pressure, temperature and stress fully coupled.

Injectivity

- **Why**
  - ▷ Common cause of sudden loss of injectivity: Hydrate formation (detrimental to downhole and surface facilities)
  - ▷ Hydrates are solid phases that form when gas mix with water at low temperatures and high pressures
- **What and how**
  - ▷ Coupled thermal-hydro-mechanical numerical simulation
  - ▷ Temperature rises back while pressure declines. The hydrates become thermodynamically unstable ("melt away")
- **Benefit**
  - ▷ Simulations can help us design an intermittent injection process – alternating between "injection" and "Shut-offs"





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Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Carbon Capture **Utilization and Storage**

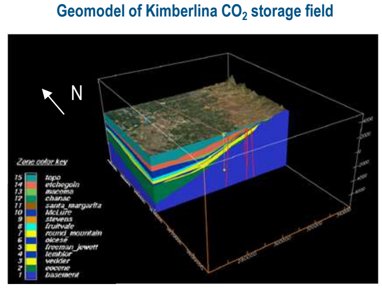
▷ Fault reactivation assessment with FEA mechanical earth model to assess risk of induced seismicity and leakage through faults.

containment

- **Why**
  - ▷ Fault reactivation can possibly compromise fault sealing capacity or induce seismic events
- **What and how**
  - ▷ Perform a geomechanical analysis for an industry-scale carbon sequestration project located in the Southern San Joaquin Basin, California USA
- **Benefit**
  - ▷ Advanced geomechanical and parallel computing capabilities
  - ▷ Simulation results show a reactivation of the faults with a limited moment magnitude
  - ▷ Moment magnitude is an output related to fault slippage and rupture area

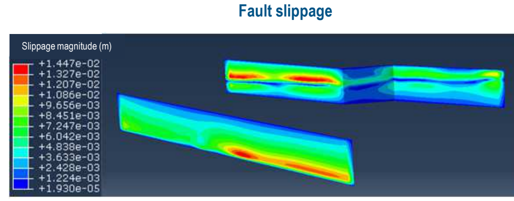
Moment magnitude
magnitude scale of seismic event

Geomodel of Kimberlina CO_2 storage field



Mechanical earth model

Fault slippage



DASSAULT SYSTEMES

Molecular and meso scale | Pore and grain scale | Core and near well bore scale | Field scale

Carbon Capture **Utilization and Storage**

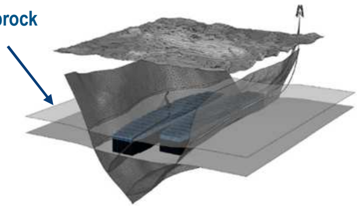
▷ Caprock integrity assessment with FEA mechanical earth model to assess risk of loss of containment by caprock failure.

containment

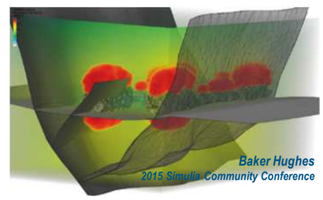
- Why
  - ▷ Caprock has a very low permeability and acts as a vertical flow barrier. It is critical for longevity and safety of CO_2 storage
- What and how
  - ▷ Perform a finite element geomechanical simulation to analyze the stress and strain behavior within the caprock
- Benefit
  - ▷ Simulations results include safe factor based on Mohr-Coulomb criterion or cumulative plastic deformation
  - ▷ These results are then used to assess the likelihood of fracture slip, which may comprise the caprock seal integrity

Safety factor based on Mohr-Coulomb criterion

Caprock



Shear stresses above the critical value (red) indicate a higher chance of fractures with the potential to CO2 leakage.



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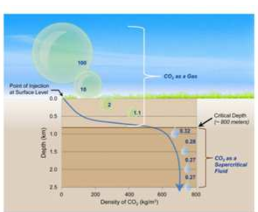
Carbon Capture **Utilization and Storage**

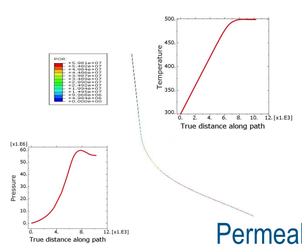
Core and near well bore scale ▷ Evolution of the thermodynamic state of the injected CO_2

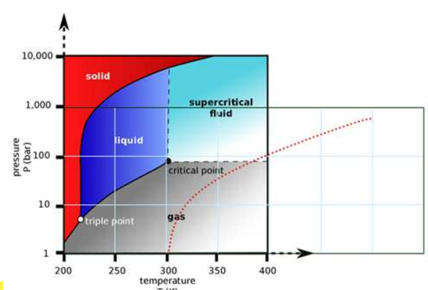
storage

Ensure long-term storage by reducing the fluid (CO_2) mobility.
By Injecting CO_2 in super-critical state (enhancing viscosity)

Simulations help us determine the required depth to keep CO_2 in super-critical state.







Permeability

Mobility $K = \kappa / \mu$

Viscosity

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70

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Carbon Capture **Utilization and Storage**

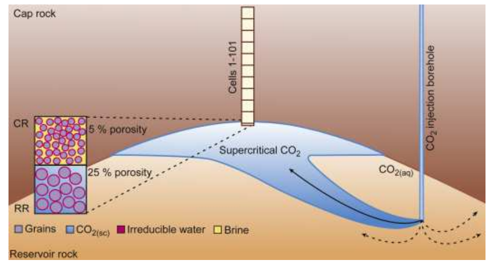
Field scale ▷ Field scale injectivity analysis with pressure, temperature and stress fully coupled to assess injectivity trends such as gradual loss of injectivity.

Injectivity

CO_2 is trapped in reservoir formation by low permeability rocks (cap-rocks)

Simulation can help us determine the spatial distribution of pressure, temperature and stresses, and their evolution in time.

- Determine the gradual loss in injectivity (filling of the porous volume)
- Inputs for the cap-rock integrity analysis.



Simulations can help determine the pressure, temp. and stresses in and around the cap-rock

Permeability

Mobility $K = \kappa / \mu$

Viscosity

71

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Carbon Capture, Utilization and Storage

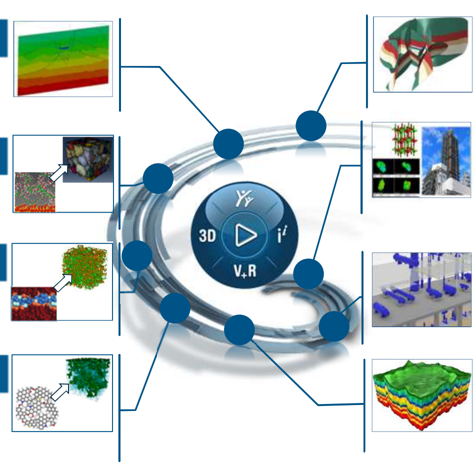
Enable Zero Carbon Emissions w/ existing Workflows

PREVENT CO2 LEAKS IN CAPROCKS
Geomechanics, Caprock Integrity

IMPROVE MODEL FIDELITY FOR INSITU CONDITIONS
DigitalROCK | Relative Permeability & Micro-mechanics

UTILIZE CO2 FOR ENHANCED OIL RECOVERY (EOR)
DigitalROCK | Relative Permeability + BIOVIA | Materials Studio

ASSESS CO2 STORAGE CAPACITY & INJECTIVITY
DigitalROCK | Absolute & Relative Permeability + BIOVIA | Materials Studio



AVOID FAULT REACTIVATION FROM CO2 INJECTION
Geomechanics | Fault Stability

INVENT NEW MATERIALS TO CAPTURE CO2
BIOVIA | Materials Studio + DigitalROCK

DESIGN PLANTS TO CAPTURE & TRANSPORT CO2
Engineering Excellence | Plant Engineering Integrity Analysis

BUILD A DIGITAL TWIN OF YOUR STORAGE SITE
Geomechanics | Wellbore Integrity

72

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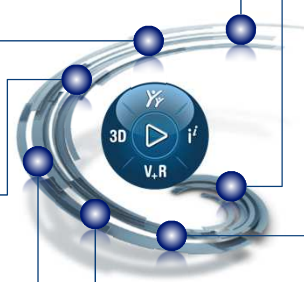
Benefits of DS Solutions for CCUS

Increase longevity and safety of CO2 storage
Geomechanics, Caprock Integrity, Wellbore Integrity

Reduce uncertainty of geological storage model
Relative Permeability
Micro-mechanics | Materials Studio, DigitalROCK

Enable effective CO2 utilization for Enhanced Oil Recovery
Relative Permeability, Fluid Flow | Materials Studio, DigitalROCK

Avoid costly mistakes and project delays by precisely assessing CO2 storage capacity and injectivity
Absolute & Relative Permeability in Media | Materials Studio + DigitalROCK



Maintain integrity and highest levels of safety of CO2 storage
Geomechanics | Fault Stability

Superior CO2 capture through new fit-for-purpose materials
Identify, Design, Optimize Materials & Process | Materials Studio + DigitalROCK

Quick, effective, safe capture and transportation of CO2
Engineering Excellence | Plant Engineering Integrity Analysis

Ability to safely simulate multiple storage scenarios by using digital twin principle
Geomechanics | Mechanical Earth Model

73

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Scope *(example)*

- DigitalROCK Relative permeability - 18 Kr curves
  - 6 MicroCTs
  - 3 Kr/MicroCT
- Molecular Dynamics Wettability - 6 wetting conditions
  - 3 fluid pairs
  - 2 surfaces (e.g. clay and quartz)
- Molecular Dynamics IFT - 3 IFT conditions
  - 3 fluid pairs

74

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