Modeling coupled processes
Solving multi-field problems with object-oriented numerical methods
Application examples in geotechnics and hydrology

Olaf Kolditz
Variety of problems
Variety of geoscientific problem requires system analysis
Outline

- **Introduction / Motivation**
  - Geotechnics
  - Hydrology, soil science

- **Governing equations**

- **Software issues**
  - Object-oriented methods
  - HPC and visualization

- **Applications**
  - CO2 sequestration
  - Nuclear waste deposition
  - Coupled hydrosystems
  - Geothermal energy (Norihiro Watanabe)
HIGRADE Course on THM Mechanics


HIGRADE Course 2011 on Reactive Transport
Continuum Mechanics
Multi-Physics: THMC coupled processes

Heat transport

\[
\frac{c_p}{\partial t} \frac{\partial T}{\partial t} = -\nabla (-K \nabla T + \sum h_\beta F_\beta) + q
\]

Thermodynamics

Mechanics

Deformation

\[
\nabla \sigma - \rho g = 0
\]

\[
\nabla \cdot \left( \sigma - (S^p p^l + S^g p^g) I - \beta T \Delta T I \right) + \rho g = 0
\]

Hydraulics

Chemistry

Reactive transport

\[
F_\kappa = \sum_\beta \left( X_\kappa F_\beta + \rho_\beta D_\kappa \nabla X_\beta \right)
\]

\[
\ln(K_{P,T}) = \frac{\Delta G_{P,T}^0}{RT}
\]

\[
K_j = \frac{a_{\nu w j} \prod_i (\gamma_i C_i)^{\nu_{i,j}} \prod_m (a_m)^{\nu_{m,j}} \prod_g (f_g)^{\nu_{g,j}}}{\gamma_j C_j}
\]
Porous Media: Phases and Components

- Micro-organisms
- Gaseous phase
- NAPL phase
- Solid phase
- Water phase
Theoretical background: Heat transport in porous media (T)

- Governing equation
  \[ \rho C_p T' = -\nabla q_T + Q_T(x, t), \quad x \in \mathbb{R}^3 \]
  \[ q_T = -K_e \nabla T + n \sum_{\gamma}^{phase} (\rho_\gamma C_p^\gamma) T v, \quad \gamma = \text{liquid, gaseous} \]

- Boundary and initial conditions
  \[ q_T \cdot n = q_\Gamma, \quad \text{or} \quad T = T_\Gamma, \quad \forall x \in \partial \Omega \]
  \[ T(x, t) = T_0(x), \quad \forall x \in \Omega \]
Theoretical background:
Non-isothermal flow in porous media (H)

Governing equation

\[ n \left[ (\rho_w - \rho_v) \frac{\partial S}{\partial p} + S \beta_p \rho_w + (1 - S) \frac{\rho_v}{\rho_w RT_{abs}} \right] \frac{\partial p}{\partial t} + \nabla \cdot (q_w + q_v) + S \rho_w \frac{\partial}{\partial t} (\nabla \cdot u) \]

\[ n(1 - S) \left( h \frac{\partial \rho_v S}{\partial T} + \frac{\rho_v p}{RT_{abs}^2} \right) \frac{\partial T}{\partial t} = 0 \]

Vapor flux: \( q_v = -D_{pv} \nabla p - f_{Tv} D_{Tv} \nabla T \)
Theoretical background:
Non-isothermal flow in porous media (H)

Boundary and initial conditions

Neumann: \( q_w \cdot \mathbf{n} = q^f, \forall \mathbf{x} \in \partial \Omega \)

Dirichlet: \( p = p_\Gamma, \quad S = S_\Gamma, \forall \mathbf{x} \in \partial \Omega \)

\[ p(\mathbf{x}, t) = p_0(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega \]
Theoretical background:
Deformation in porous media (M)

- Governing equation

\[ \nabla \cdot (\sigma - SpI) + \rho g = 0 \]
\[ \sigma = C \Delta \epsilon^e = C (\Delta \epsilon - \alpha \Delta T I) \]

- Boundary and initial conditions

\[ \sigma : n = t \quad \text{or} \quad u = u_{\Gamma}, \quad \forall \mathbf{x} \in \partial \Omega \]
Constitutive theory

Wang, Görke et al. (2007-10)

The total Cauchy stress tensor in porous media is decomposed in partial stresses referring to the participating phases.

\[
\mathbf{\sigma} = (1 - n) \mathbf{\sigma}^s - n \left( \sum_\gamma S^\gamma p^\gamma \right) \mathbf{I}
\]

Attention:
Note the sign convention of positive fluid phase pressure \( p^\gamma \), but negative compressive normal stress for the solid phase!

Effective solid stress

Modification of the stress representation

\[
\mathbf{\sigma} = \mathbf{\sigma}_E^s - \left( \sum_\gamma S^\gamma p^\gamma \right) \mathbf{I} \quad \text{with} \quad \mathbf{\sigma}_E^s = (1 - n) \left[ \mathbf{\sigma}^s + \left( \sum_\gamma S^\gamma p^\gamma \right) \mathbf{I} \right]
\]

Effective solid stress:
Total solid stress reduced by the excess pore liquid pressure, but referred to the domain of the overall porous medium.
Constitutive theory

Generalized material classes

Experimentally observed rate-independent solid material behavior. Cyclic uniaxial stress-strain curves: without hysteresis (left), with hysteresis (right)

Experimentally observed rate-dependent solid material behavior. Cyclic uniaxial stress-strain curves: without hysteresis (left), with hysteresis (right)
Material classes – Mathematical models

According to the experimental observations, there are four classes of mathematical models matching the material classes defined above:

- Theory of elasticity describes rate-independent material behavior without hysteresis
- Theory of (elasto)plasticity describes rate-independent material behavior with hysteresis
- Theory of viscoelasticity describes rate-dependent material behavior without hysteresis
- Theory of viscoplasticity describes rate-dependent material behavior with hysteresis

Classification of material behavior depends on real loading regime (e.g. small or large strains), environmental conditions (e.g. temperature), and the time scale of the physical processes under consideration.
Constitutive theory

Material classes – Physico-mathematical substitute models

Physically significant constitutive relations in the uniaxial case can be defined for material classes based on so-called rheological models (simple networks of individual rheological elements)

Individual rheological elements

\[ \sigma = k \varepsilon \]
\[ \sigma = \eta \dot{\varepsilon} \]
\[ \varepsilon = \begin{cases} 0, & \text{if } \sigma < \sigma^* \\ \varepsilon(t), & \text{if } \sigma \geq \sigma^* \end{cases} \]
Governing Equations

Media and solid constitutive assumptions

- All phases are assumed to be materially incompressible
  \([\rho^{sR}, \rho^{lR}, \rho^{CO_2R}: \text{const}]\)

- Capillary pressure definition:
  \([p^c = p^{CO_2} - p^l]\)

- Brooks-Corey’s model characterizing hydraulic properties
  
  - Relative permeability functions
    \[
    k_{rel}^{l} = (S_{eff})^{(2+3\lambda)/\lambda} \quad \text{with} \quad S_{eff} = \frac{S^l - S_{res}^l}{1 - S_{res}^l - S_{res}^{CO_2}}
    \]
    \[
    k_{rel}^{CO_2} = (1 - S_{eff})^2 \left(1 - (S_{eff})^{(2+\lambda)/\lambda}\right)
    \]

  - Capillary pressure saturation relation
    \[
    S_{eff} = \left(\frac{p^D}{p^c}\right)^{\lambda}
    \]

- Homogeneous isotropic elastic solid skeleton
Böttcher et al. (2010)

EOS
Equations of state

Span&Wagner EOS, 1996
GOVERNING EQUATIONS

H³ Problem

Diffusive wave surface flow

\[
\phi_a \frac{\partial H_a}{\partial t} + \nabla \cdot \mathbf{q}^{of} = q_s^{of} \\
0 \leq \phi_a \leq 1
\]

\[
q^{of} = -\frac{CH^{l+1}}{S_s^{1+j}} \nabla h^{of}
\]

Richards flow in soil

\[
\phi \frac{\partial S}{\partial t} + \nabla \cdot \mathbf{q}^{sf} = q_s^{sf}
\]

\[
q^{sf} = -k_r K \nabla (\Psi + z)
\]

Groundwater flow in aquifer

\[
\phi \frac{\partial h^{gf}}{\partial t} + \nabla \cdot \mathbf{q}^{gf} = q_s^{gf}
\]

\[
q^{gf} = -K \nabla h^{gf}
\]

Jens-Olaf Delfs

Borden Aquifer
OK et al. (JHI 2008)
Computational Mechanics
Finite element approach:
Weak forms with the test function

\[ \omega \in \mathcal{V} \subset H_1^1(\Omega) \]

\( \nabla \text{balance equation (T)} \ 
\int \int_\Omega \beta \left( \sigma - S \rho \mathbf{I} \right) : \left( \nabla \omega + (\nabla \omega)^T \right) \ d\Omega - \int \int_\Omega \omega^T \cdot \rho \mathbf{g} \ d\Omega \]

\(- \int \int_\Gamma \omega^T \cdot \mathbf{t} \ d\Gamma = 0 \)

\(+ \int \int_\Omega n (1 - S) \left( \frac{\partial \rho_v}{\partial T} + \frac{\rho_v p}{RT_{abs}^2} \right) \frac{\partial T}{\partial t} \omega \ d\Omega = 0 \)
Finite element approach:
Applying the Galerkin method to the weak forms leads to the coupling equations

- Thermal and hydraulic equations
  \[ M_T T' = -K_T T + f_T(p) \]
  \[ M_f p' = -K_f p + f_f(T, u) \]

- Mass and Laplace matrices
  \[ M = \int_{\Omega} N M N^T \, d\Omega, \quad K = \int_{\Omega} \nabla N K (\nabla N)^T \, d\Omega \]

- Mechanical equation
  \[ \int_{\Omega} B^T D B \, d\Omega u = f(p, T) \]
Finite element approach:
The derived coupling equations are solved in the problem-dependent staggered/monolithic manner.

Heat emitting waste  CO2
Numerical Methods - Summary

- Weak formulations based on the method of weighted residuals
- Spatial discretization: standard Galerkin finite element method
- Time discretization: generalized first order difference scheme
- Picard linearization of the nonlinear coupled boundary value problem
- Primary variables: $p^c$, $p^{CO_2}$, $u^s$ (alternat.: $p^l$, $S^{CO_2}$, $u^s$)
- Equations of twophase flow processes solved in monolithic manner (pressure-pressure scheme; $p^c$, $p^{CO_2}$)
- Coupling to deformation processes by staggered iterations (partitioned approach)
- Realization: object oriented scientific in-house code OpenGeoSys
- Verified by several classical benchmarks (e.g. Buckley-Leverett, McWorther, Liakopoulos)
OO Software Concept
HPC Developments and Applications
**Multi-Physics: THMC coupled processes**

### Heat transport

\[
c_\rho \frac{\partial T}{\partial t} = -\nabla (-K \nabla T + \sum_\beta h_\beta \vec{F}_\beta) + q
\]

### Fluid flow

\[
\frac{\partial}{\partial t} \int_{V_n} M^\kappa dV_n = \int_{\Gamma_n} \vec{F}^\kappa \vec{n} d\Gamma_n + \int_{V_n} q^\kappa dV_n
\]

\[
M^\kappa = \Phi \sum_\beta \rho_\beta S_\beta X_\beta^\kappa
\]

\[
\vec{F}_\beta^\kappa = -\rho_\beta \frac{k_{kr_\beta}}{\mu_\beta} (\nabla P_\beta - \rho_\beta \vec{g})
\]

\[
\sum_\beta S_\beta = 1
\]

### Thermodynamics

### Mechanics

\[
\nabla \sigma - \rho \vec{g} = 0
\]

\[
\nabla \cdot \left( \sigma - \left( S^d p^d + S^g p^g \right) \mathbf{I} - \beta T \Delta T \mathbf{I} \right) + \rho g = 0
\]

### Hydraulics

### Chemistry

### Reactive transport

\[
\vec{F}^\kappa = \sum_\beta \left( X_\beta^\kappa \vec{F}_\beta + \rho_\beta \vec{D}_\beta^\kappa \nabla X_\beta^\kappa \right)
\]

\[
\ln(K_{P,T}) = \frac{\Delta G_{P,T}^0}{RT}
\]

\[
K_j = \frac{a_{w_j} \Pi_i (\gamma_i C_i)^{\nu_i,j} \Pi_m (a_m)^{\nu_m,j} \Pi_g (f_g)^{\nu_{g,j}}}{\gamma_{j} C_j}
\]
Version 4: Object-Orientation for Multifield Problems

Geometry
Points
Polylines
Surfaces
Volumes
Domains

Topology
NOD Nodes
ELE Meshes

MFP
MSP
MMP
MCP
MAT
PCS
GEO
NUM
EQS
MSH

IC
BC
ST

Source code reduction: 10 (V3) -> 3 MB (V4)

Ax = b
x = A⁻¹b

CProcess::Create()
CProcess::Config()
CProcess::Execute()

J Hydroinformatics
Version 4.4 – OO-FEM

**OO-ELE**

**Element Objects**

\[ A_{ij}(x_j)x_i = b_i \]

\[
K^e = \int_{\Omega^e} \nabla N^T \frac{1}{\mu} \nabla N^T d\Omega^e \\
= \int_{-1}^{+1} \int_{-1}^{+1} \int_{-1}^{+1} \frac{1}{\mu} \frac{\mathbf{J}^{-1} \mathbf{T}^{T} \mathbf{J}^{-1} \mathbf{T}^{T} \mathbf{K}^{T} \mathbf{J}^{-T} \mathbf{N}^{T} \mathbf{J} \mathbf{N}}{\det(J)} d\mathbf{r} d\mathbf{r} d\mathbf{r}
\]

**inline void CFiniteElementPCS::LaplaceMATFunction**

\{ 
    switch(m_pcs->type) {
        case L: // Liquid flow
            case G: // Gas flow
                case T: // Two phase flow
                    case C: // Componental flow
                        case R: // Richards flow
                            tensor = m_mmp->PermeabilityTensor(Index);
                            mat_fac = m_mmp->PermeabilitySaturationFunction() \n                                / mfp_vector[0]->Viscosity();
                            for(i=0; i<ele_dim; i++)
                                mat[i] = tensor[i] * mat_fac;
                            break;
                        case H: // Heat transport
                            case M: // Mass transport
                                case D: // Deformation
                                    break;
                }
            }
    }

Wang & Kolditz (2007)
J Num Methods Eng
• MPI parallelization

\[ A^0_{ij} x^0_j \rightarrow h^0_I \]

\[ A^1_{ij} x^1_j \rightarrow h^1_I \]

\[ \ldots \]

\[ A^n_{ij} x^n_j \rightarrow h^n_I \]

\[ (h^0_0, h^0_1, h^0_2, h^0_3, \ldots, h^n_{\text{dim}_\text{loc}}) \]

Sorted sparse table

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<th>Node/Row</th>
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<th>5</th>
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</tbody>
</table>

Version 4.5 – MPI-FEM
**MPI-Efficiency for THM coupled problems**

- **Class: SparseTable**
  - Constructor(...) // by mesh data
  - Constructor(...) // by subdomain mesh data
  - private:
    - Store sparsity pattern as described in
  - public:
    - Return the pointer of this class

- **Class: SparseMatrix**
  - Constructor(...) // by SparseTable instance
  - private:
    - Pointer to SparseTable
    - DOF per node
    - An array of non-zero entries
  - public:
    - Operators for matrix computation

**Wenqing Wang**

- **Fig. 20. Temperature distribution after 45 years**

- **Fig. 21. Vertical stress after 100 years**
MPI-Efficiency for THM coupled problems
MPI-Efficiency for THM coupled problems
• OpenMP parallelization

Test bed (8 x DualCore)

• Hybrid parallelization (GRID computing)

Simple test example
HPC Platforms

Super-Computer

- SX6 (HLRS)
  0.3 TFlop/s
- SX8 (HLRS)
  15 TFlop/s
- Cray XT3 (PSI)
  8.5 TFlop/s, 1664 CPUs
- BlueGene/L (FZJ)
  Test node

Linux Cluster

- LiClus (UFZ)
  256 CPUs (QuadCore)
- Strider (HLRS)
  256 Opteron CPUs
- Merlin 3 (PSI)
  256 Opteron CPUs
- HYDRA (ZAG)
  8 AMD Opteron CPUs
Flexibility of OO codes, but ...

THMC coupling

Surface/subsurface coupling

Fracture networks

OpenMP

MPI
Monte-Carlo simulation on Parallel Clusters

Norihiro Watanabe

Measurements

Scenario / Assumptions

Statistical property of sample data

Stochastic reservoir model

Virtual reservoir1

Virtual reservoir2

... Virtual reservoir N

Parallelization

THM model

THM model

THM model

Prediction1

Prediction2

... Prediction N

Data analysis
(Parallel) Threading for Root-Soil Systems

Thomas Kalbacher

Start Interface
  Configure

Parent
  do fork()

Child (1/root)
Child (1)

Simulation Time Speed-Up with MPI

Processing Time

- Sun Fire X4600 (Infiniband)
- Opteron 248 Cluster (Gusabt Ethernet)

G E O S Y S: Parallel Version

a R O O T: Serial Version

Ω_1 Ω_2 Ω_3 \ldots Ω_n
Ω_n+1 Ω_n+2 Ω_n+3 Ω_n+m

Technische Universität Dresden
Helmholtz Centre for Environmental Research – UFZ
Geochemical Simulators Coupled to OGS

- World wide distributed Aquatic geochemistry
- Low T, low C, kinetic
- Free code

- PHREEQC
- EQLink
- CHEMAPP
- MultiComp
- Transport
- Special Data for nuclide Thermodynamics
- Sorption & desorption
- Uncertainty

- Biogeochemical Microbiological processes

- BRNS
- GEMS

- Flexible Thermodynamics (High T, high C)
OGS Focus - Reactive Transport

HIGRADE Course 2011: Reactive Transport
Maintenance of scientific software - OpenSource

(6 Partners from 4 countries
In all about 100 people)
Plattform-independent: CMake
Automated benchmarking: CTest
Scientific Visualization 3D data explorer: Qt
TESSIN - Helmholtz Topic Center
for Terrestrial Environmental System Simulation and INtegration

Data modeling
High performance computing
Scientific visualization

Water resources
Geotechnics (CO2)
Geothermal energy
Landscape modeling
Process Understanding
Benchmarks / Code comparison
Real Applications
Multiphase flow ($H^2$)
Chan-Hee Park, Wenqing Wang
3D multiphase flow

Chan-Hee Park
Known Numerical Issues and Workarounds: Multiphase flow

- **Local mass conservatory method**
  - Finite difference method
  - Finite volume method
  - Mixed-finite element method

- **Non-local mass conservatory method**
  - Standard Galerkin finite element method
Primary Variables: Multiphase flow

- Oil science: $P_w$ and $P_{nw}$
- Soil science: $P_c$ and $P_{nw}$
- Water resources science: $P_w$ and $S_w$ or $S_{nw}$
H²(\(P_w S_{nw}\) and \(P_c P_{nw}\) ): Kueper’s Experiment - Heterogeneity (Water and Oil)

Selection of primary variables ... don’t forget about physics
Is CO₂ wetting or non-wetting to media of our interests?
Multiphase flow ($H^2T$)
Non-isothermal effects
Norbert Böttcher, Ashok Singh
Test case definition for supercritical fluids (Böttcher et al. 2010)

\[
\frac{\partial S_\alpha}{\partial t} = \frac{\partial p_\alpha}{\partial t} = \frac{\partial T}{\partial t} = 0
\]

\[
S_{CH_4}(x_0, t) = 0
\]
\[
p_{CO_2} = 7.55 \text{ MPa}
\]
\[
T(x_0, t) = 300 \text{ K}
\]

\[
S_{CH_4}(x, t_0) = 0.99
\]
\[
p_{CH_4} = 7.5 \text{ MPa}
\]
\[
T(x, t_0) = 400 \text{ K}
\]
Non-isothermal effects for supercritical fluids

(Böttcher et al. 2010)
Multiphase flow consolidation (H²M)
Defining test cases
Joshua Taron, Uwe Görke
Known Numerical Issues and Workarounds:
Conversion of primary variables on nodal points to cell centers or the other way around

- What if mechanical deformation is involved?
  - Merge of FEM and FVM or FDM
A benchmark proposal for $H^2M$ - Definition

Model description

- Synthetic scenario at real storage site (Ketzin, Germany)
- Deep aquifer fully saturated with saline water
- Radius of injection well: 0.2 m, radius of the domain: 200 m
- Initial stress: rock pressure due to gravitational forces
- Constant Neumann boundary condition for the injection rate
- Material parameters/properties taken from literature

CO2 Injection model

Axisymmetric model of CO$_2$ injection into deep saline aquifer analyzing near-field liquid spreading

Triangular mesh for finite element analyses
H²M: German test site for CO₂ storage in deformable media

**Fluid properties**

<table>
<thead>
<tr>
<th>Term</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Saline water density</td>
<td>kg/m³</td>
<td>1173</td>
</tr>
<tr>
<td>Saline water viscosity</td>
<td>Pa·s</td>
<td>1.252×10⁻³</td>
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<tr>
<td>Residual water saturation</td>
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<tr>
<td>Maximum water saturation</td>
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<td>0.95</td>
</tr>
<tr>
<td>CO₂ density</td>
<td>kg/m³</td>
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<tr>
<td>CO₂ viscosity</td>
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<tr>
<td>Residual CO₂ saturation</td>
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</tr>
<tr>
<td>Maximum CO₂ saturation</td>
<td>-</td>
<td>0.65</td>
</tr>
</tbody>
</table>

**Medium properties**

<table>
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<th>Unit</th>
<th>Value</th>
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</thead>
<tbody>
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<td>Intrinsic Permeability</td>
<td>m²</td>
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<tr>
<td>Brook-Corey's index</td>
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<td>2.0</td>
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<tr>
<td>Porosity</td>
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<tr>
<td>Entry pressure</td>
<td>Pa</td>
<td>10⁴</td>
</tr>
<tr>
<td>Young's modulus</td>
<td>Pa</td>
<td>2.0×10¹¹</td>
</tr>
<tr>
<td>Poisson ratio</td>
<td>-</td>
<td>0.3</td>
</tr>
</tbody>
</table>
A benchmark proposal for H²M - Results

Temporal evolution of the CO₂ saturation in two selected points

Temporal evolution of tangential effective stresses in two selected points
A benchmark proposal for H²M - Results

Spatial distribution of the CO₂ saturation within the domain 1 and 1000 hours respectively after injection started.

Spatial distribution of tangential effective stresses within the domain 1 and 1000 hours resp. after injection started.
Multiphase flow consolidation (H²M)
Shear slip during CO2 injection
**H^2M Problem Definition:**

- **Line source of CO_2 injection:** 500 tones per year
- **Vertical cross-section at 3 km depth**
- **Shale**
  - \( \sigma_v = 76.5 \text{ MPa} \)
  - \( \sigma_h = 0.6 \sigma_v \)
  - \( \Delta x = 1 \text{ m} \) and \( \Delta z = 0.5 \text{ m} \)
- **Sandstone**
  - \( q_{nw}(50,1) = 1.87 \times 10^{-3} \text{ m}^3/\text{day} \)
  - \( \{ p_w = 31 \text{ MPa and } S_{nw} = 0 \} \) or \( \{ p_c = 19 \text{ kPa and } p_{nw} = p_w + p_c \} \)
CO$_2$ Saturation with 20 Years of the Injection

The PwSnw Model

- 1 year
- 10 years
- 20 years
- 100 years

The PcPnw Model

- 1 year
- 10 years
- 20 years
- 100 years

S(CO$_2$)

0.841 0.561 0.280 0.000

0.645 0.464 0.282 0.100
Safety Factors for Shear Slip Failure: The realistic failure mode

The PwSnw Model

1 year
10 years
20 years
100 years

The PcPnw Model

(a)
(b)
A systematic for CO2 benchmarking #1 Processes

<table>
<thead>
<tr>
<th>Problem type</th>
<th>Process type</th>
<th>Dimension</th>
<th>DBB</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compressible flow</td>
<td>H</td>
<td>1-D</td>
<td>7</td>
</tr>
<tr>
<td>Two-phase flow (Buckley-Leverett)</td>
<td>$H^2$</td>
<td>1-D</td>
<td>20.3</td>
</tr>
<tr>
<td>Two-phase flow (McWorther-Sunada)</td>
<td>$H^2$</td>
<td>1-D</td>
<td>20.4</td>
</tr>
<tr>
<td>Two-phase flow (Keuper)</td>
<td>$H^2$</td>
<td>2-D</td>
<td>20.5</td>
</tr>
<tr>
<td>Unsaturated consolidation</td>
<td>HM</td>
<td>2-D</td>
<td>14.3</td>
</tr>
<tr>
<td>Two-phase flow consolidation</td>
<td>$H^2M$</td>
<td>2-D</td>
<td>14.4</td>
</tr>
<tr>
<td>Thermo-mechanics</td>
<td>TM</td>
<td>2-D / 3-D</td>
<td>15</td>
</tr>
<tr>
<td>Non-isothermal compressible flow</td>
<td>TH</td>
<td>1-D</td>
<td>7</td>
</tr>
<tr>
<td>Non-isothermal two-phase flow</td>
<td>$TH^2$</td>
<td>1-D</td>
<td>17</td>
</tr>
<tr>
<td>Non-isothermal unsaturated consolidation</td>
<td>THM</td>
<td>2-D</td>
<td>16</td>
</tr>
<tr>
<td>Non-isothermal two-phase flow consolidation</td>
<td>$TH^2M$</td>
<td>2-D</td>
<td>17</td>
</tr>
</tbody>
</table>

Table 1
Benchmarks by processes
A systematic for CO2 benchmarking #3 Scenarios

Table 3
Benchmarks by sites and scenarios.

<table>
<thead>
<tr>
<th>Problem type</th>
<th>Process type</th>
<th>Dimension</th>
<th>Doc</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ketzin</td>
<td>H²</td>
<td>2-D(r)</td>
<td>Sec. 3.1</td>
</tr>
<tr>
<td>Altmark</td>
<td>THC²</td>
<td>2-D(r)</td>
<td>Sec. 3.2</td>
</tr>
<tr>
<td>Svalbard</td>
<td>H²/M</td>
<td>2-D</td>
<td>Sec. 3.3, [3]</td>
</tr>
<tr>
<td>Stuttgart</td>
<td>H²</td>
<td>3-D</td>
<td>Sec. 3.4, [2]</td>
</tr>
<tr>
<td>Shear slip</td>
<td>H²M</td>
<td>2-D</td>
<td>see TV III.2.2-1, this report</td>
</tr>
</tbody>
</table>

(a)
Multiphase flow consolidation (TH²M)
Non-isothermal effects
DECOVALEX-IV Task D

Development of COupled models
And their VAlidation against EXperiments

Task D – Teams:
DOE/LBNL  Lawrence Berkeley National Laboratory
CAS        Chinese Academy of Science
JAEA/JNC   Japan Atomic Energy Agency
           Japan Nuclear Cycle Development Inst.
           Hazama Corporation
BGR/UFZ    Federal Institut for Geosciences
           Helmholtz Center for
           Environmental Sciences
THM1/2 Task Definitions

<table>
<thead>
<tr>
<th>Repository design</th>
<th>D_THM1 (FEBEX Type)</th>
<th>D_THM2 (Yucca Mountain Type)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model Height, Lz (m)</td>
<td>1,000</td>
<td>500</td>
</tr>
<tr>
<td>Drift spacing, Lx (m)</td>
<td>35</td>
<td>51</td>
</tr>
<tr>
<td>Drift Diameter, D (m)</td>
<td>2.28</td>
<td>5.5</td>
</tr>
<tr>
<td>Maximum thermal line load, Pw (W/m)</td>
<td>245 (at emplacement)</td>
<td>592 (at 50 years)*</td>
</tr>
</tbody>
</table>

* Heat load is reduced by drift ventilation until 50 years after emplacement
Geomechanical Processes
Short-Term Effects

Significant geomechanical effects are expected in response to heat release from the decaying radioactive waste

FEBEX type:
- Drying / wetting of bentonite induces shrinkage and swelling in the buffer

Yucca Mountain type:
- High temperature dryout zone by boiling effects

Thermally induced stresses will act upon rock mass:
- thermal expansion effects might be recoverable but ...
Geomechanical Processes  
Long-Term Effects

- thermal stresses may lead to irreversible impacts

Changes in the stress field during the heating period can lead to inelastic mechanical response induced by fracture shear slip or crushing of fracture asperities

Elevated temperatures and stresses will be maintained for long time periods -> increased microcracking, crack growth -> irreversible changes in hydraulic properties
THM Simulations - T Process

THM1-FEBEX

THM1-YuccaMountain

Forced Ventilation

V3 (At drift wall)

V6

Power (W/m)

Power (W/m)

TEMPERATURE (°C)

TEMPERATURE (°C)

TIME (Years)

TIME (Years)

(a) Profiles for t ≤ 100 years

(b) Profiles for t ≥ 1,000 years

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Page 70
THM Simulations - M Process
THM Simulations - H Process

THM1-FEBEX

THM1-YuccaMountain

Stress dependent permeability changes for Yucca Mountain type
## THM Teams – Flow models

<table>
<thead>
<tr>
<th>Team</th>
<th>Numerical Simulator</th>
<th>Hydraulic Model</th>
<th>Treatment of Buffer Swelling</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOE</td>
<td>TOUGH-FLAC</td>
<td>Multiphase liquid and gas flow</td>
<td>NA</td>
</tr>
<tr>
<td>DOE</td>
<td>ROCMAS</td>
<td>Single-phase unsaturated liquid flow with thermal vapor diffusion in static gas phase</td>
<td>Linear swelling strain model as a function of water saturation (targeted to give 5 MPa at full saturation*)</td>
</tr>
<tr>
<td>BGR</td>
<td>GeoSys/ Rockflow</td>
<td>Basic model with single-phase unsaturated liquid flow and thermal vapor diffusion and alternative multiphase flow model for comparison</td>
<td>Alternative swelling model as a function of water saturation (possibly not targeted for 5 MPa)</td>
</tr>
<tr>
<td>CAS</td>
<td>FRT-THM</td>
<td>Single-phase unsaturated liquid flow with thermal vapor diffusion in static gas phase</td>
<td>Linear swelling strain model as a function of water saturation (targeted to give 5 MPa at full saturation)</td>
</tr>
<tr>
<td>JAEA</td>
<td>THAMES</td>
<td>Single-phase unsaturated liquid flow with thermal vapor diffusion in static gas phase</td>
<td>Alternative swelling model as a function of water saturation (possibly not targeted for 5 MPa)</td>
</tr>
</tbody>
</table>

* The target pressure of 5 MPa was specified in the task description (Barr et al., 2005).
Richards vs Two-Phase Flow

Special Issue (2009)
Non-isothermal flow in low permeable porous media: a comparison of Richards’ and two-phase flow approaches

Wenqing Wang · Jonny Rutqvist · Uwe-Jens Görke · Jens T. Birkholzer · Olaf Kolditz

\[ \frac{\partial p^c}{\partial y} = \frac{\partial p^g}{\partial y} = 0 \]

\[ T = 120^\circ C \]
\[ \frac{\partial p^c}{\partial x} = \frac{\partial p^g}{\partial x} = 0 \]

\[ p^c(\vec{x}, t) \bigg|_{t=0} = 75\text{MPa}, \quad T(\vec{x}, t) \bigg|_{t=0} = 30^\circ C \]
\[ \frac{\partial p^c}{\partial x} = \frac{\partial p^g}{\partial x} = 0 \]

\[ \frac{\partial p^c}{\partial y} = \frac{\partial p^g}{\partial y} = 0 \]

\[ 0.1 \text{ m} \]

Fig. 1 Numerical model of the CTF1 experiment
**Richards vs Two-Phase Flow**

**Intrinsic permeability**

- $10^{-13} \text{m}^2$
- $10^{-18} \text{m}^2$
Reactive Transport
Results of THC Simulations

1D-Test

Mineral Abundances

IC: liquid saturation

Temperature (°C)

IC for pore water chemical and mineral compositions for both materials

BC:

Left point: heat source (T=T(0) (=THC heat power times 1/16))

Right end point: liquid saturation 1.0, T=24.6°C, granite pore water in equilibrium at 24.6°C
Richards vs.
Two-Phase-Flow Models

Figure 20: Alteration of Annite and Pyrite, Multiphase flow / Richards flow
- Reactive nuclide transport
- 120 species have to be considered to represent the geochemical system
- non-ideal solid solutions
- 60 in PSI data base

Reactive Transport
Nuclear Waste Deposition

Haibing Shao (PhD thesis 2010)
Approaching the Reality

Geometry matters ...

Björn Zehner, Lars Bilke
HPC in real applications of THM codes

Whiteshell URL
Canada
HPC in real applications of THM codes
HPC in real applications of THM codes
Presentation
Norihiro
Watanabe

Geothermal reservoir simulation
BENCHMARKING

Benchmarking projects in CO2 storage: CO$_2$BENCH
Hydrology: H$^N$BENCH
Geothermics: GEOBENCH
Conclusions

- **Community efforts are necessary ...**
  - Observation & Data assimilation
  - Conceptual modelling
  - Numerical methods
  - Computer sciences
  - Open source philosophy
  - Transparent and efficient work platforms
  - Cooperation between NLs and Universities
  - ...

- **Computer power & man power ...**
  - more complexity must coincide with a better understanding
  - ...

Thank you for your attention
Hydrology II

TERENO
www.tereno.net
Bode Model

Work flow

ACCESS → ORACLE → OGS-DE → GMS → OGS-FEM → mHM

Database

Karsten Rink Feng Sun
SELKE CATCHMENT
First results

Wenqing Wang
Luis Samaniego
Jens Delfs

mHM: Groundwater recharge

OGS: Groundwater discharge
Hydrology I

Yajie Wu
10^6 grid nodes

Density-dependent flow