Mathematical and Numerical Modelling of Multiphase and Multicomponent Flow in Heterogeneous Media

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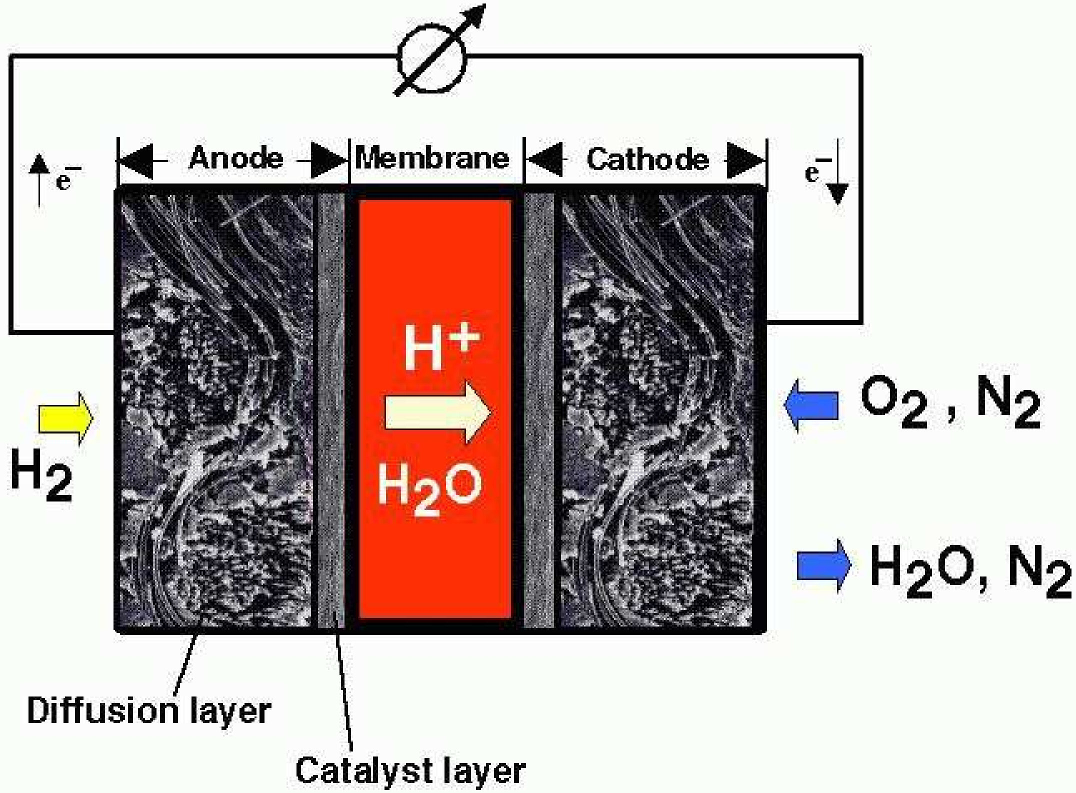
Multiphase Processes in a Fuel-Cell



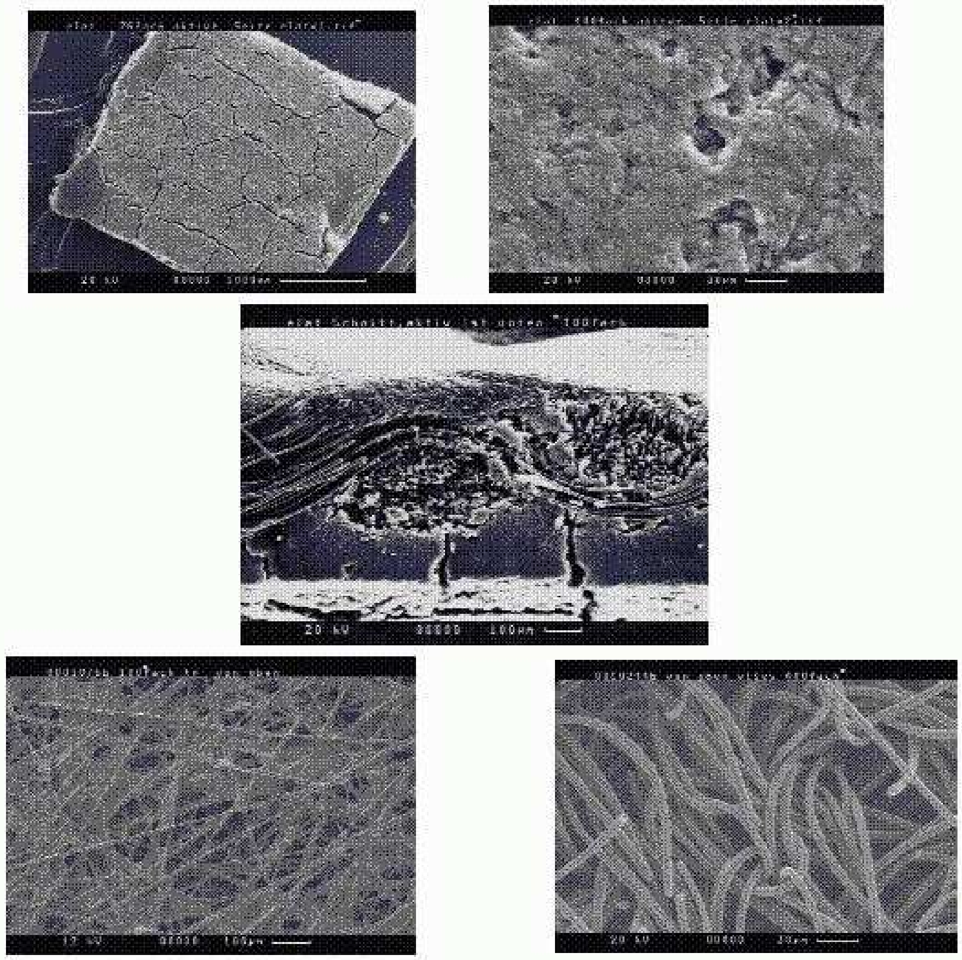
$H_2 \rightarrow 2H^+ + 2e^-$ $\qquad$ $2H^+ + 2e^- + \frac{1}{2} O_2 \rightarrow H_2O$

- fuel-cell operation at
  50 - 80°C
  1 - 2 bar (g)
- vapor-saturated air
- liquid water appears at the cathode

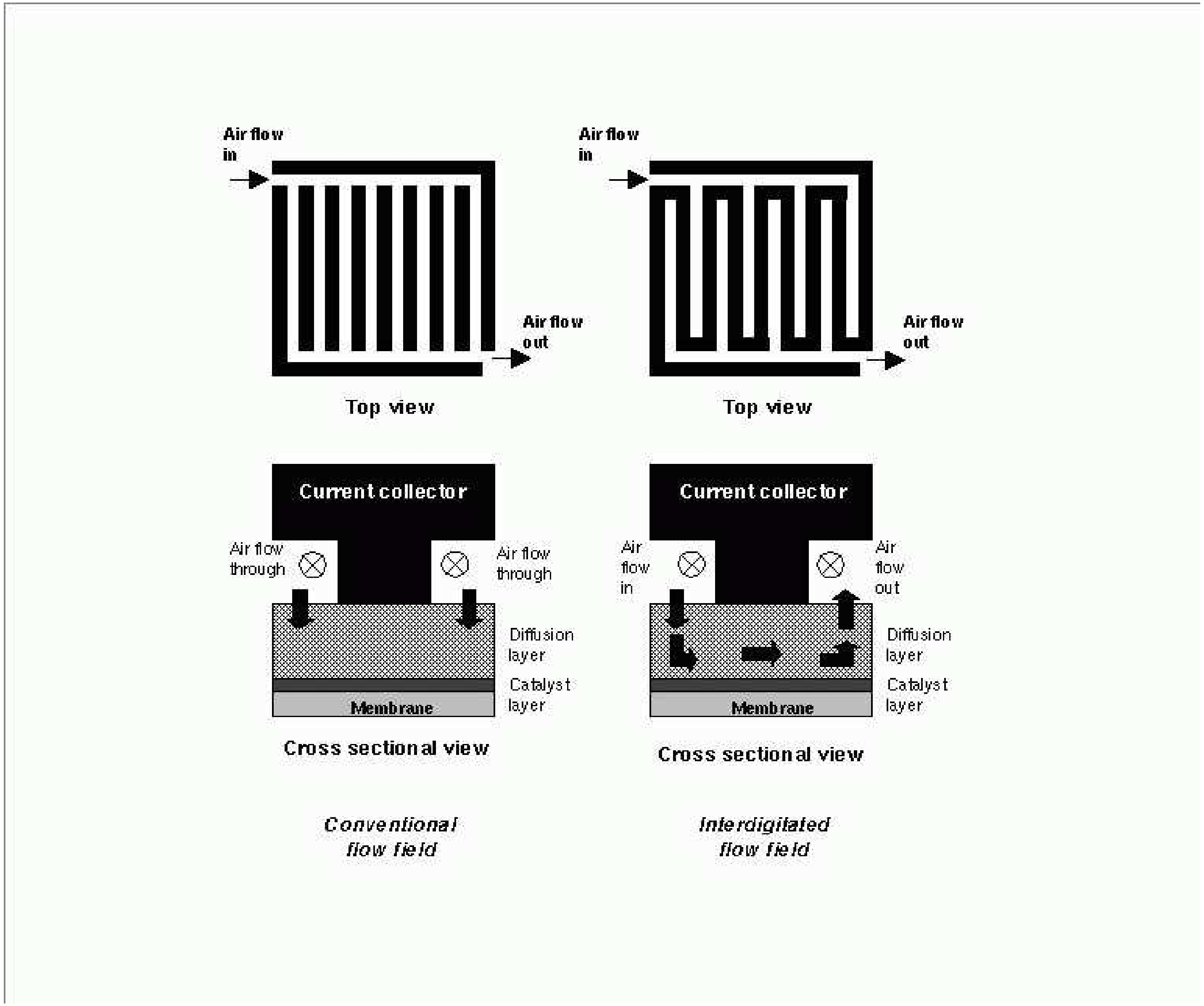
Diffusion Layer and Flow-Field Plate

- performance of the fuel-cell is strongly influenced by the properties of the diffusion layer and the flow-field plate.
- diffusion layer
  - protection of the membrane
  - distribution of the gases
  - liquid water transport
  - electric contact
- commonly used media for the diffusion layer
  - hydrophobic carbon cloth, fleece or paper
- gas current collector
  - gas supply
  - water transport
  - electric contact
- common materials
  - metal plates or graphite plates with incorporated profiles

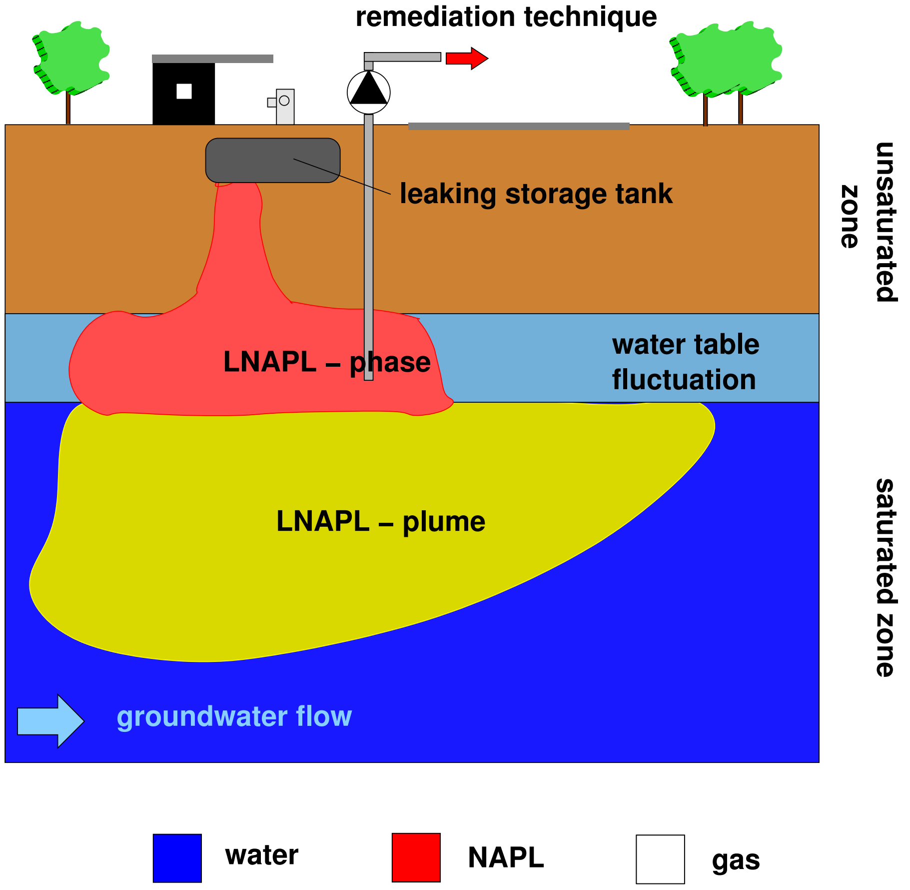
Diffusion Layer



Gas Current Collector

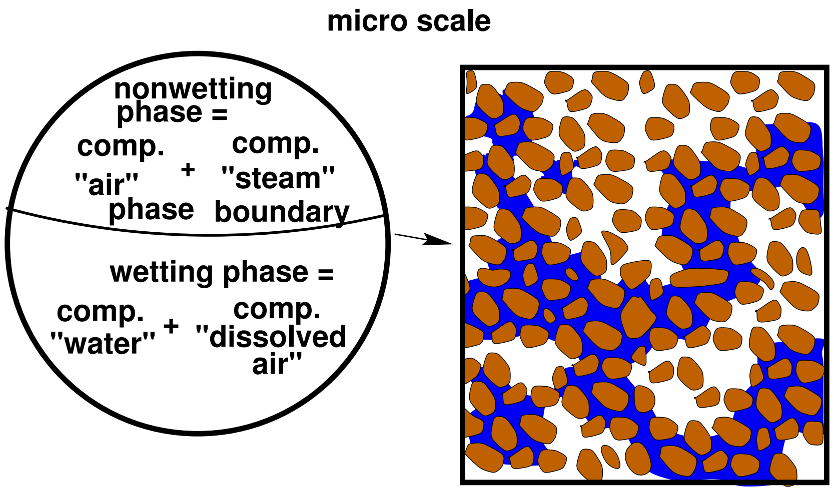


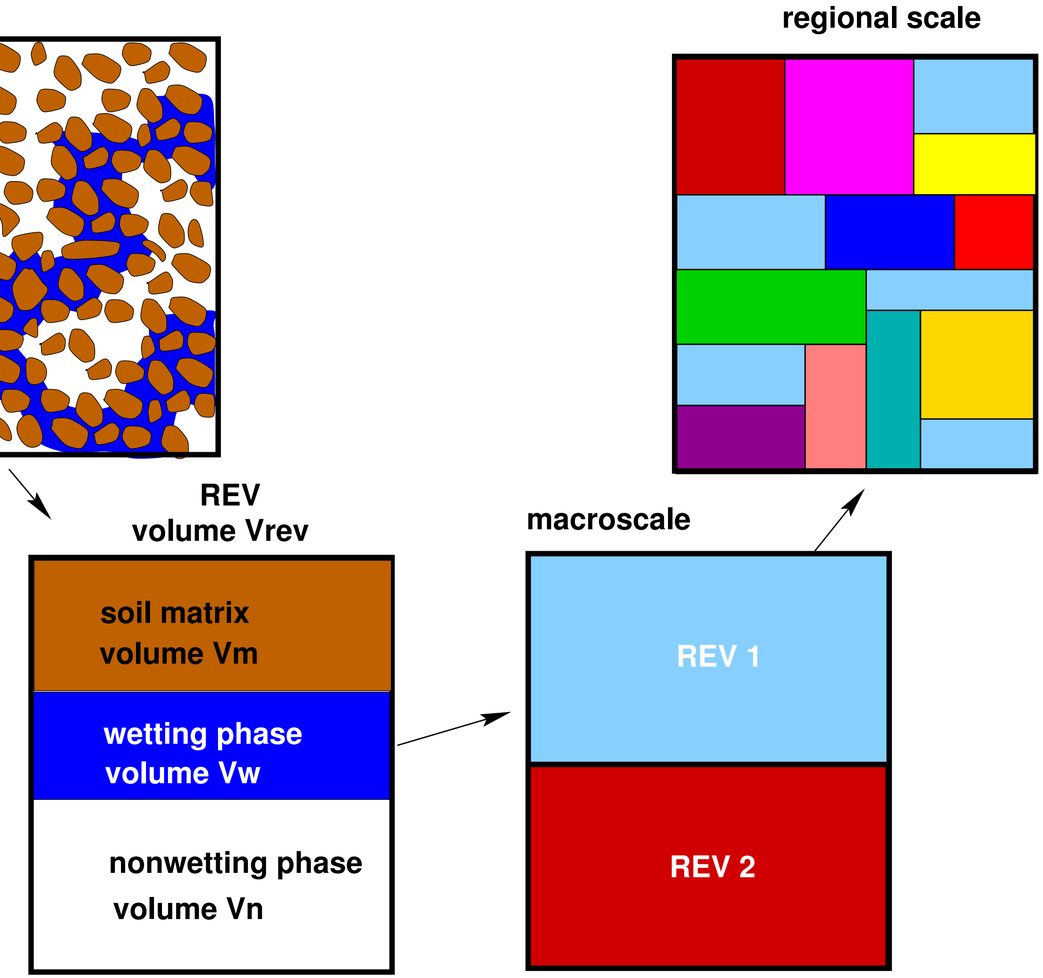
LNAPL spill into the subsurface



- Infiltration of LNAPL into the subsurface
- Formation of a separate contaminant phase
- Plume of dissolved LNAPL
- Contamination of groundwater aquifers

Scales and REV



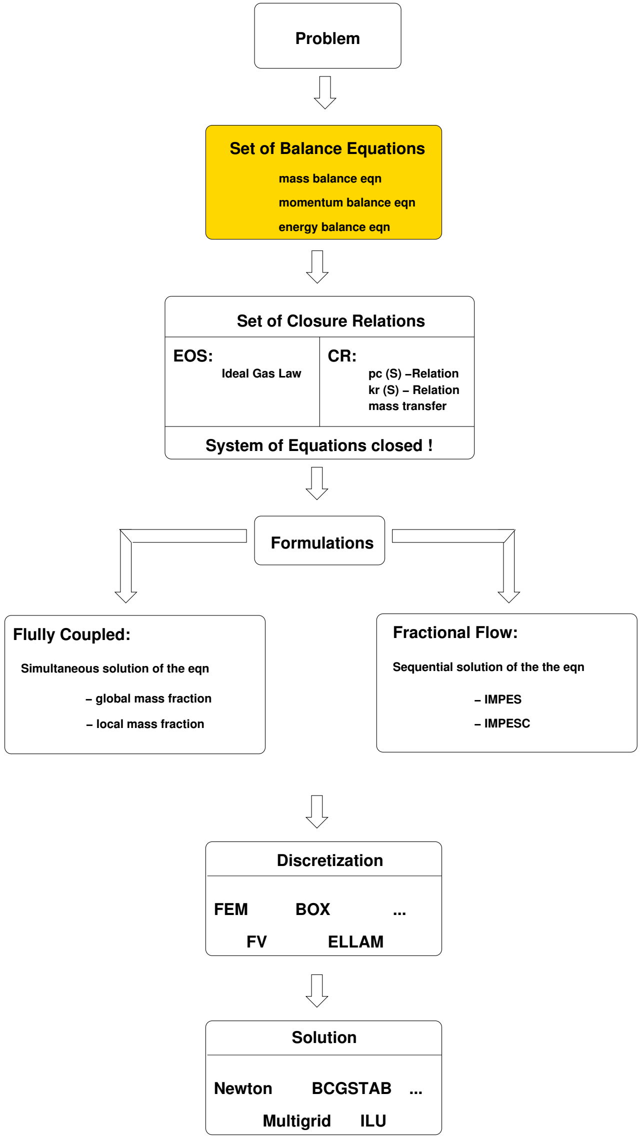


porosity $\phi = \frac{Vw + Vn}{Vrev}$

saturation of the wetting phase $Sw = \frac{Vw}{Vw + Vn}$

saturation of the nonwetting phase $Sn = \frac{Vn}{Vw + Vn}$

Balance Equations for Multiphase Systems



Multiphase System

Continuum Balance equations for phase α:

1) Mass balance equation:

$$\frac{\partial(\phi S_\alpha \varrho_\alpha)}{\partial t} + \nabla \cdot (\varrho_\alpha \mathbf{v}_\alpha) = 0$$

2) Momentum balance equation:

$$\frac{\partial(\varrho_\alpha \mathbf{v}_\alpha)}{\partial t} + \nabla \cdot (\varrho_\alpha \mathbf{v}_\alpha \mathbf{v}_\alpha + \sigma_\alpha) - \varrho_\alpha \mathbf{F}_\alpha = 0$$

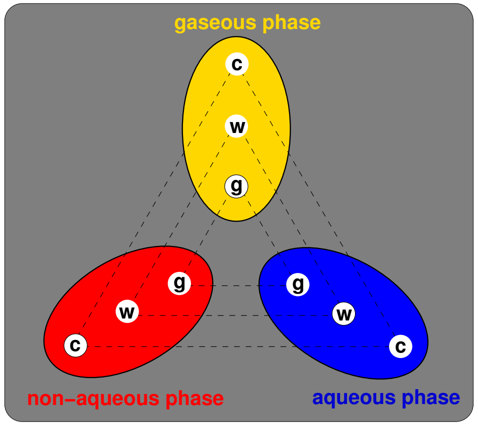
several simplifying assumptions [Bear and Bachmat (1986)]

$\Rightarrow$ Extended Darcy Law:

$$\mathbf{v}_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha} \mathbf{K} \cdot (\nabla p_\alpha - \varrho_\alpha \mathbf{g})$$

Environmental Compositional Models

General Compositional Model:



- General contaminant migration model
- All three components may partition between each phase
- Each phase exists of a major component

Compositional System

1) Mass conservation of components $K = w, c, a$:

$$\underbrace{\phi \frac{\partial(\varrho_{w_{mol}} X_w^K S_w + \varrho_{g_{mol}} X_g^K S_g + \varrho_{n_{mol}} X_n^K S_n)}{\partial t}}_{1}$$

$$- \underbrace{\operatorname{div}\left\{\frac{k_{rw}}{\mu_w}\varrho_{w_{mol}} X_w^K \mathbf{K}(\operatorname{\mathbf{grad}} p_w - \varrho_{w_{mass}}\mathbf{g})\right\}}_{2} - \underbrace{\operatorname{div}\left\{\frac{k_{rg}}{\mu_g}\varrho_{g_{mol}} X_g^K \mathbf{K}(\operatorname{\mathbf{grad}} p_g - \varrho_{g_{mass}}\mathbf{g})\right\}}_{3}$$

$$- \underbrace{\operatorname{div}\left\{\frac{k_{rn}}{\mu_n}\varrho_{n_{mol}} X_n^K \mathbf{K}(\operatorname{\mathbf{grad}} p_n - \varrho_{n_{mass}}\mathbf{g})\right\}}_{4} + \underbrace{\operatorname{div}\left\{D_{pm}^K \varrho_{g_{mol}} \operatorname{\mathbf{grad}} X_g^K\right\}}_{5} - \underbrace{q^K}_{6} = 0$$

$$D_{pm}^K = \tau \phi S_g D_g^K \qquad (D_g^K \text{ from binary diffusivities})$$

$$\rightsquigarrow D_g^w = \frac{1 - X_g^w}{\frac{X_g^a}{D_g^{aw}} + \frac{X_g^c}{D_g^{cw}}} \quad \text{and} \quad D_g^c = \frac{1 - X_g^c}{\frac{X_g^w}{D_g^{cw}} + \frac{X_g^a}{D_g^{ac}}}$$

2) Energy balance (component h):

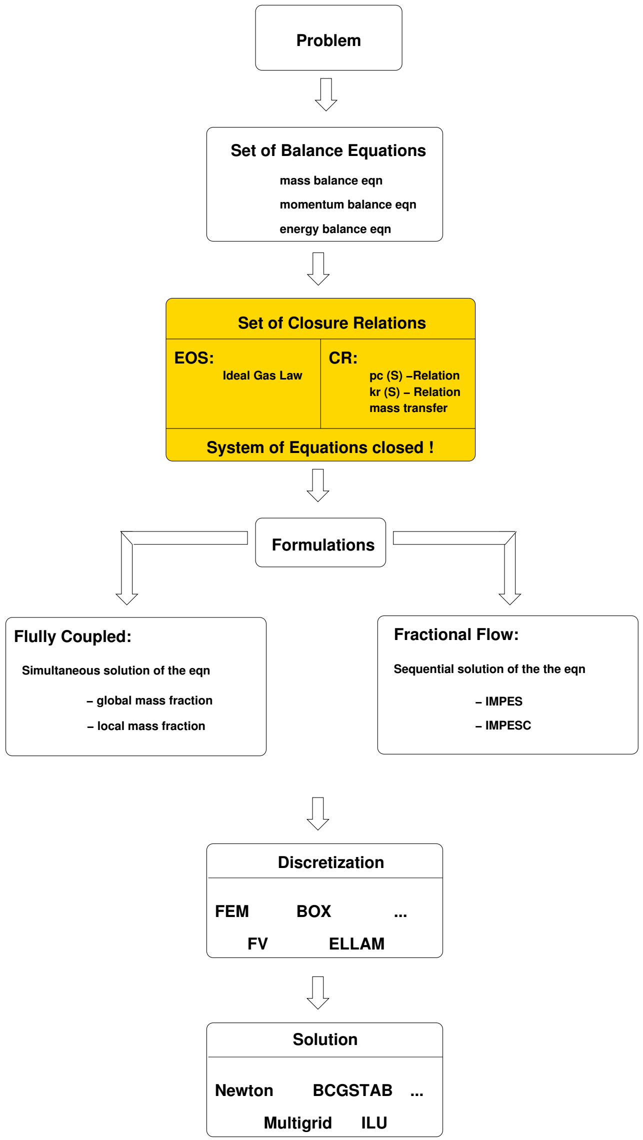
$$\underbrace{\phi \frac{\partial(\varrho_{w_{mass}} u_w S_w + \varrho_{g_{mass}} u_g S_g + \varrho_{n_{mass}} u_n S_n)}{\partial t}}_{1} + \underbrace{\frac{\partial(1-\phi)\varrho_R C_R T}{\partial t}}_{2} - \underbrace{\operatorname{div} \lambda_{pw} \,\mathbf{grad}\, T}_{3}$$

$$- \underbrace{\operatorname{div} \left\{ \frac{k_{rw}}{\mu_w} \varrho_{w_{mass}} h_w \mathbf{K} (\,\mathbf{grad}\, p_w - \varrho_{w_{mass}} \mathbf{g}) \right\}}_{4} - \underbrace{\operatorname{div} \left\{ \frac{k_{rg}}{\mu_g} \varrho_{g_{mass}} h_g \mathbf{K} (\,\mathbf{grad}\, p_g - \varrho_{g_{mass}} \mathbf{g}) \right\}}_{5}$$

$$- \underbrace{\operatorname{div} \left\{ \frac{k_{rn}}{\mu_n} \varrho_{n_{mass}} h_n \mathbf{K} (\,\mathbf{grad}\, p_n - \varrho_{n_{mass}} \mathbf{g}) \right\}}_{6} - \underbrace{\operatorname{div} \left\{ D_{pm} \varrho_{g_{mol}} h_g^w M_{wt}^w \,\mathbf{grad}\, X_g^w \right\}}_{7}$$

$$+ \underbrace{\operatorname{div} \left\{ D_{pm} \varrho_{g_{mol}} h_g^a M_{wt}^a \,\mathbf{grad}\, X_g^a \right\}}_{8} + \underbrace{\operatorname{div} \left\{ D_{pm} \varrho_{g_{mol}} h_g^c M_{wt}^c \,\mathbf{grad}\, X_g^c \right\}}_{9} - \underbrace{q^K}_{10} = 0$$

Closure Relations for Compositional Systems



Compositional System

3) Closure realtions:

a) Saturation constrains:

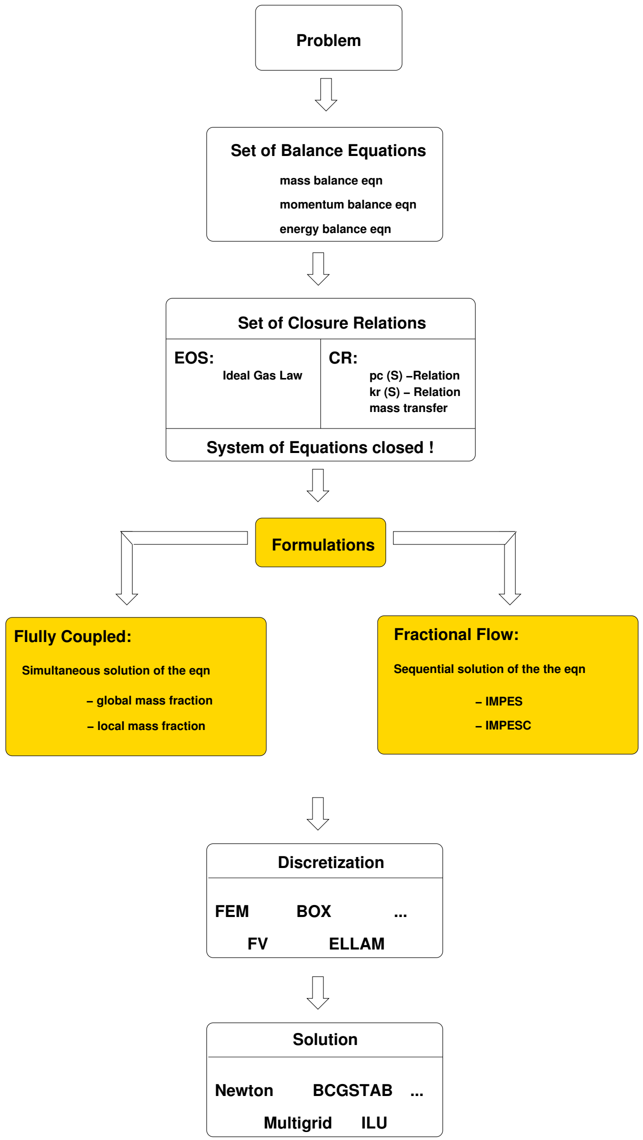
$$S_w + S_g + S_n = 1$$

b) Closure Relations:
(pc according to Lenhard and Parker, 1988)

$$\begin{aligned} p_n &= p_g - \Theta p_{c_{gn}}(S_g) - (1-\Theta)[p_{c_{gw}}(S_w) - p_{c_{nw}}(S_w = 1)] \\ p_w &= p_n - \Theta p_{c_{nw}}(S_w) - (1-\Theta)[p_{c_{nw}}(S_w = 1)] \\ \Theta &= min(1, \frac{S_n}{S_{nr}}) \end{aligned}$$

Θ is a scaling factor for a continuous transition from three-phase to two-phase systems

Formulations



Formulations

1) Fully coupled formulation

- Characterised by choice of primary variables (e.g. p_w-S_n, p_n-S_w ...)
- Simultaneous solution of the set of equations

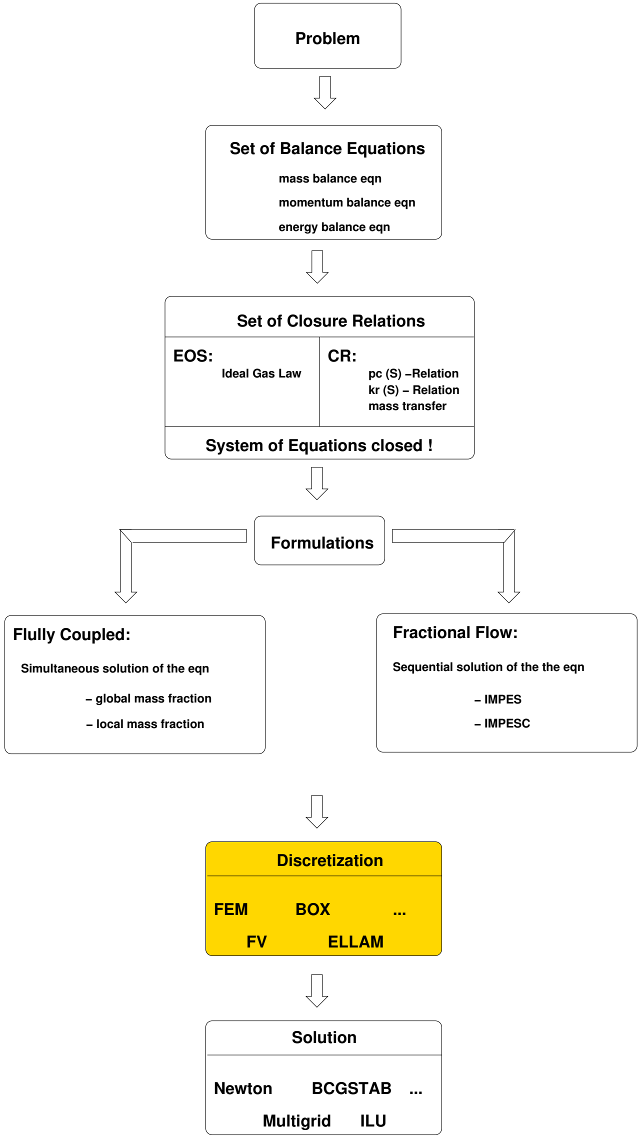
1. Phase mole or mass fractions
   - Phase mole or mass fractions as primary variables
   - Variable switching usually necessary if phase disappears
   - Alternatively a minimal saturation is introduced
2. Global mole or mass fractions
   - Global mole or mass fractions introduced
   - No variable switching necessary
   - Hard to define physical correct boundary conditions

Formulations

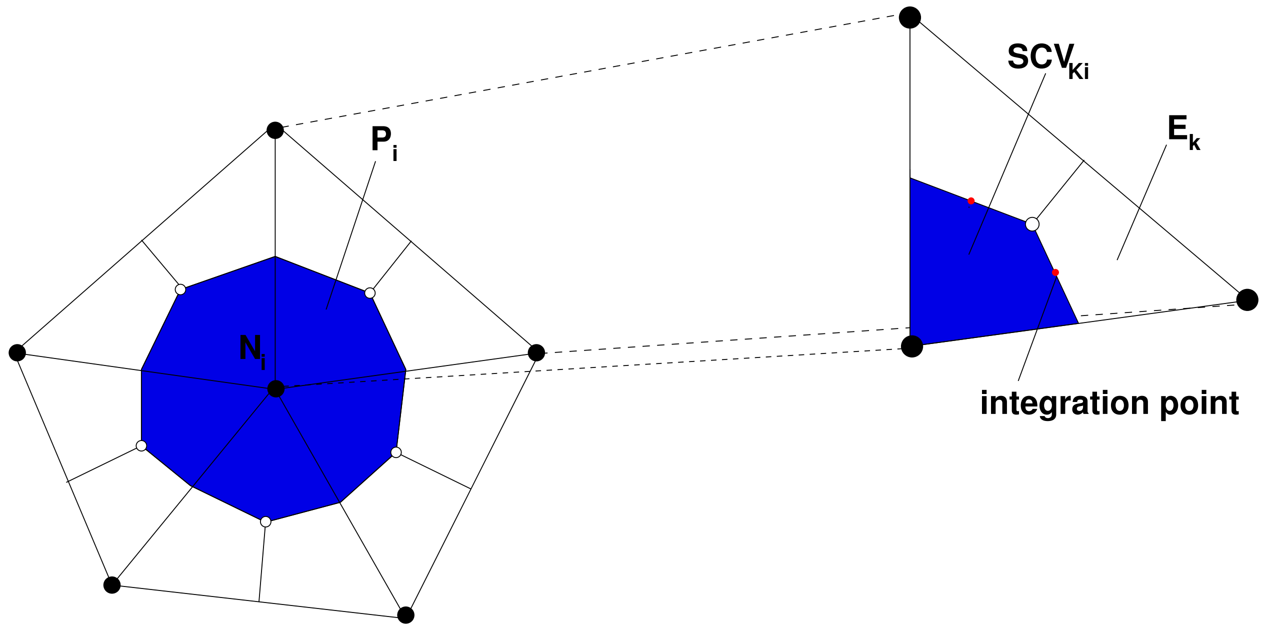
2. Weakly coupled formulation

- Introduction of global pressure and fractional flow function
- Sequential solution of the set of equations
- Implizit solution of pressure equation
- Explizit solution of Saturation Component balance eqn

Discretization

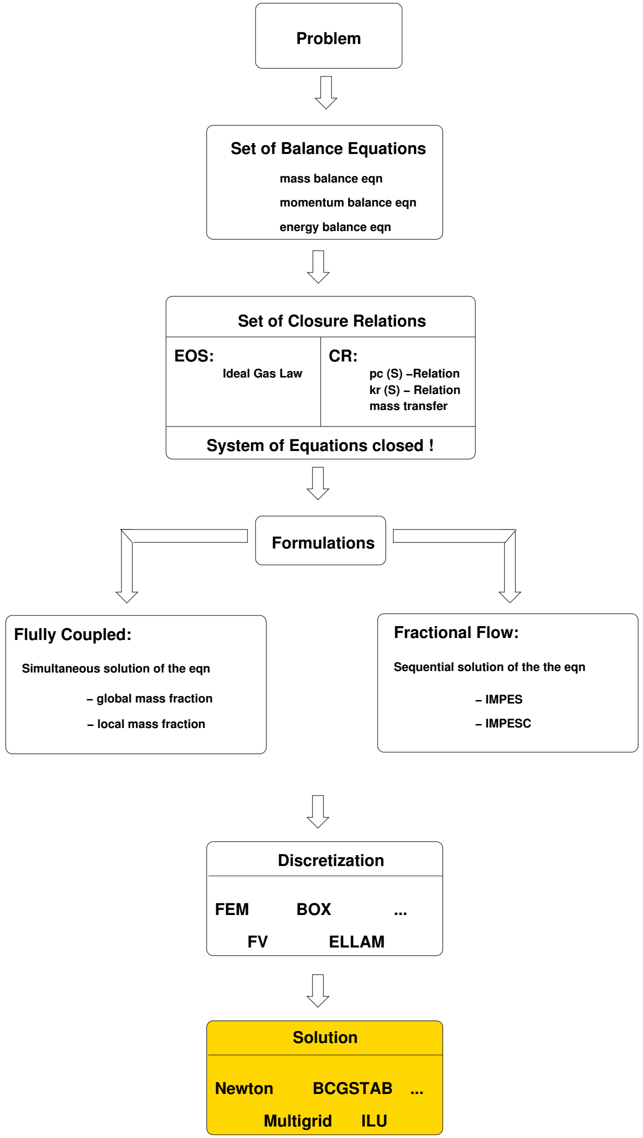


BOX Method



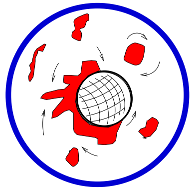
$$\underbrace{\frac{\partial}{\partial t}\int_{V_E} M^{(\alpha,k)}\,dV_E}_{mass\quad accumulation\quad term} = \underbrace{\int_{\Gamma_E} F^{(\alpha,k)}\,n\,d\Gamma_E}_{flux\quad term} + \underbrace{\int_{V_E} q^{(\alpha,k)}\,dV_E}_{source\quad term}$$

Solution Methods



MUFTE_UG

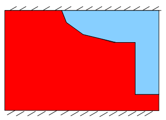
(Helmig et. al 1997, 1998)
(Bastian et. al 1997, 1998)

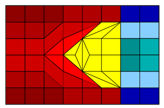


(S. Lang, K. Birken,
K. Johannsen et. al 1997)

Institute for Hydraulic Engineering (IWS)

- problem description
- constitutive relationships
- physical-mathematical models
- discretization methods
- numerical schemes
- refinement criteria
- physical interpretation

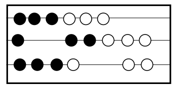


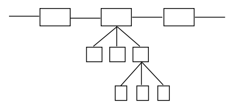


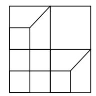
MUFTE (Helmig)

Interdisciplinary Center for Scientific Computing (IWR)

- multigrid data structures
- local grid refinement
- solvers (multigrid, etc)
- r,h,p-adaptive methods
- parallelization
- user interface
- graphic representation

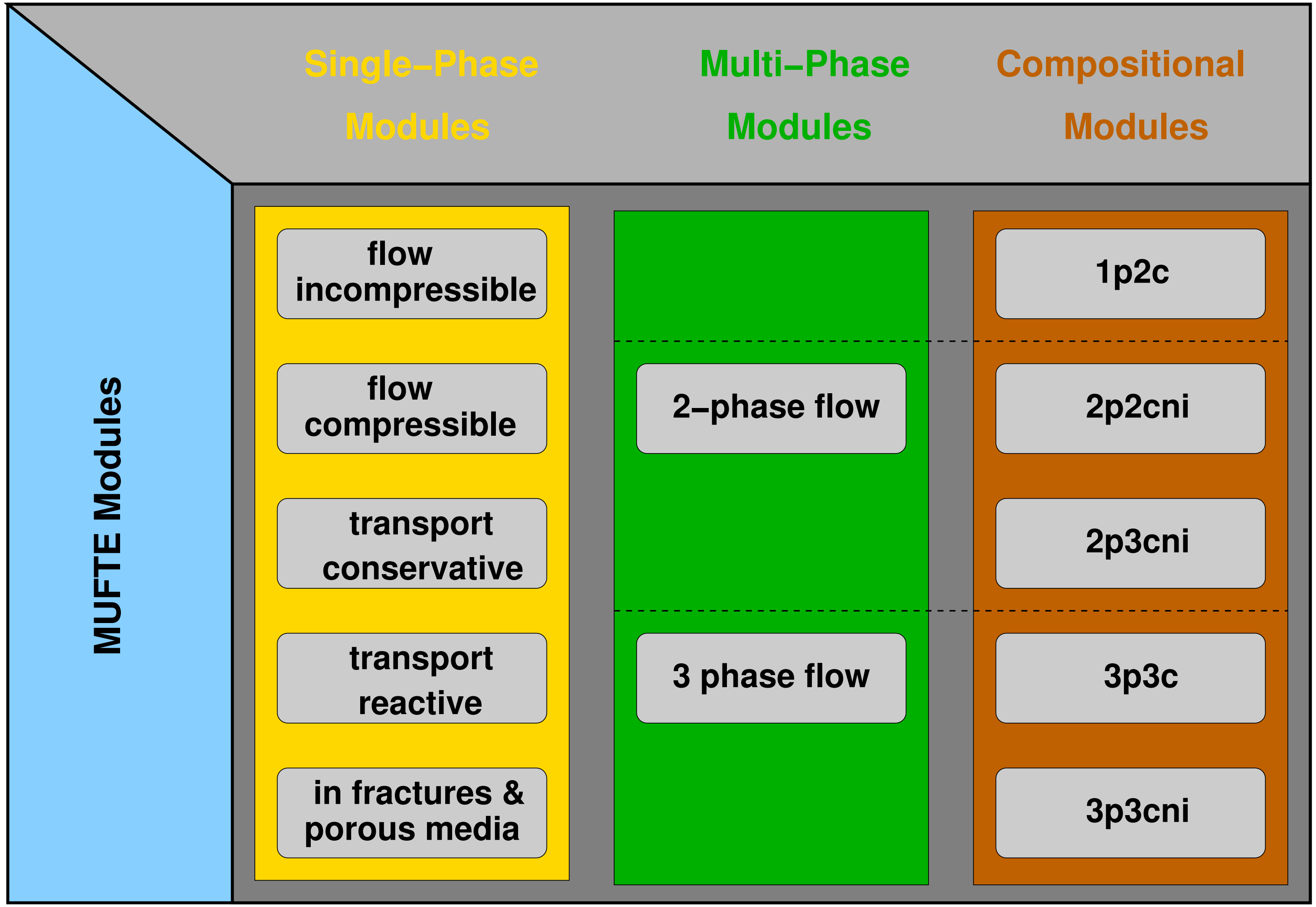






UG (Wittum, Bastian)

MUFTE-Modules



MUFTE, 2–phase modules

2p:

- Two phases, no mass transfer between phases
- Different formulations available: $p_w - S_n$, $p_n - S_w$, $p_w - p_n$
- 2D and 3D calculations possible
- Example: Buckley-Leverett problem

2p2cni:

- Two phases, two components, mass transfer between phases
- 2D and 3D calculations possible
- Example: CO_2–injection in geological formations

2p3cni:

- Two phases, three components, mass transfer between phases
- 2D and 3D calculations possible
- Example: freshwater, salt water and methane interaction processes

Formulations and Discretization Techniques (MUFTE-UG)

Formulations:

- Phase pressure and global pressure in two phase systems
- Multiphase-multicomponent isothermal and nonisothermal
- Interface conditions built in at media discontinuities

Discretization Method:

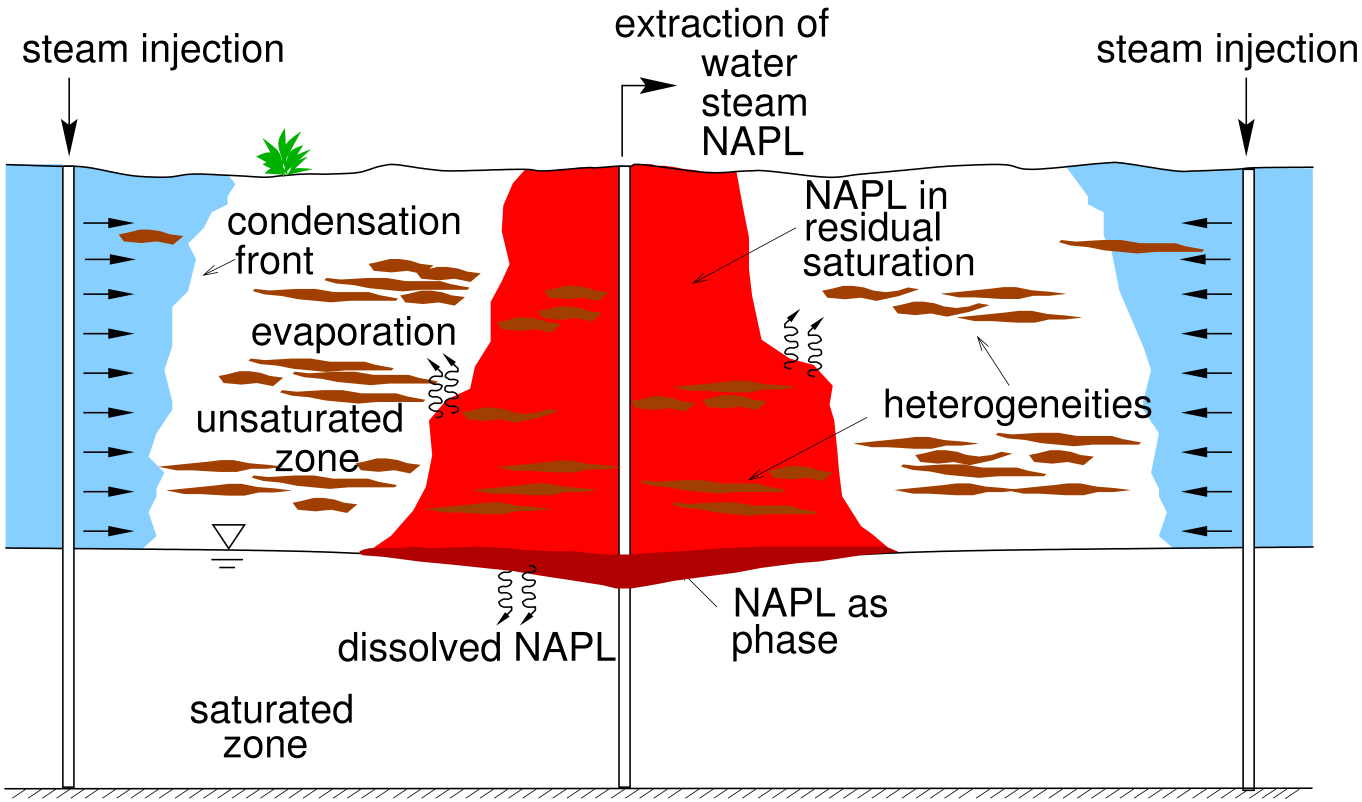
- Box formulation
- CVFE formulation
- Mixed-hybrid formulation
- Discontinuous Galerkin formulation

Solver Techniques:

- Fully coupled Newton linearization, line search globalization, nested iteration
- Fully coupled BiCGSTAB-Multigrid for arising linear systems

(Helmig, Bastian, Class, Hinkelmann, Huber, Jakobs, Sheta, 1998)

Thermally Enhanced Soil Vapor Extraction

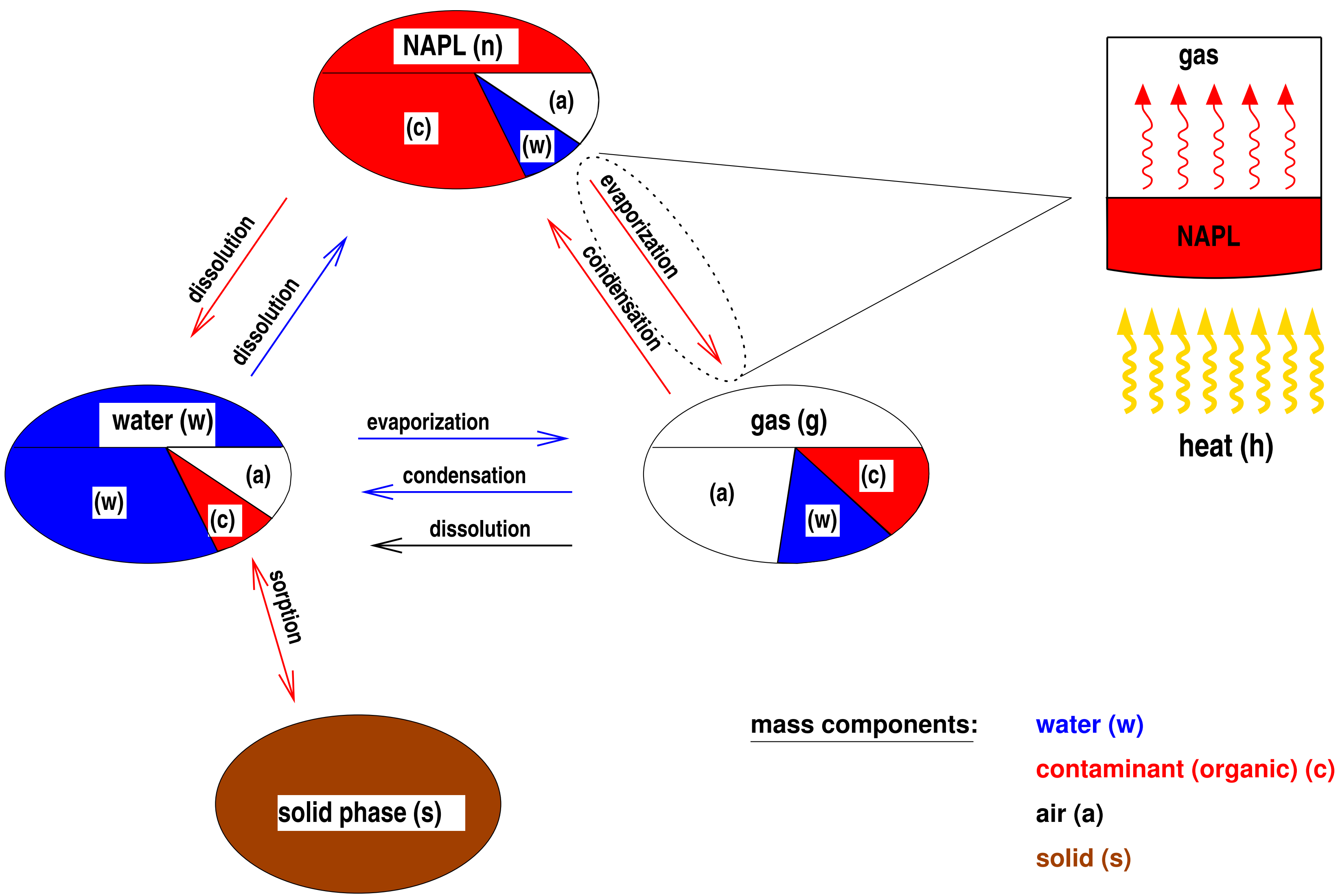


- 3-Phase 3-Component nonisothermal Model
- Fully Coupled formulation of system
- Discretization BOX Scheme

Thermally Enhanced Soil Remediation Technology

- Steam injection with soil vapor extraction
- Condensation front
- Heat transport by steam flux
  - $\leadsto$ more NAPL can evaporate
  - $\leadsto$ reduction of viscosity, surface tension and capillary forces
  - $\leadsto$ immobile NAPLs can be remobilized
  - $\leadsto$ also less permeable zones can be reached

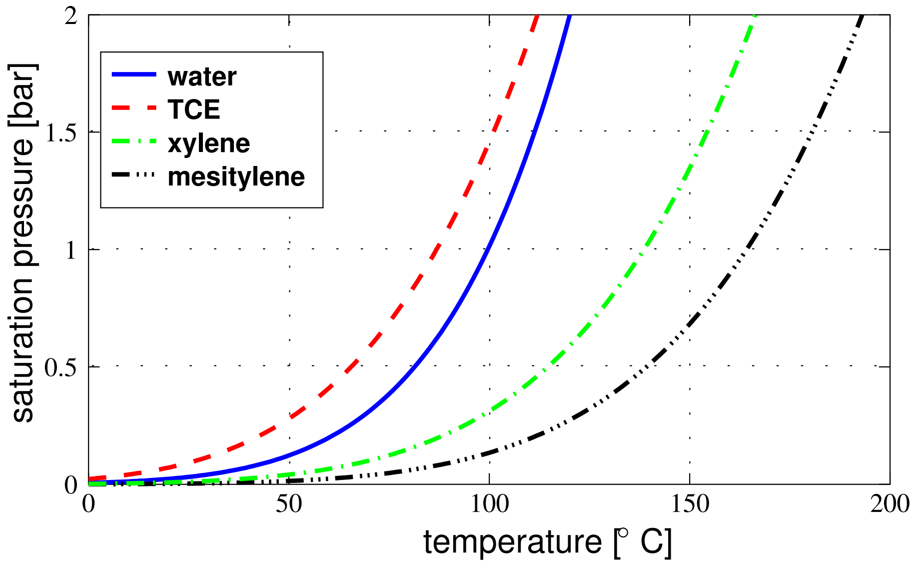
Compositional System



mass components: water (w)
contaminant (organic) (c)
air (a)
solid (s)

Phase Composition – Mole Fractions

Saturation pressure curves



Gas phase:

Dalton's Law,
Ideal Gas Law

$$x_g^w = \frac{p_g^w}{p_g}, \qquad x_g^c = \frac{p_g^c}{p_g}$$

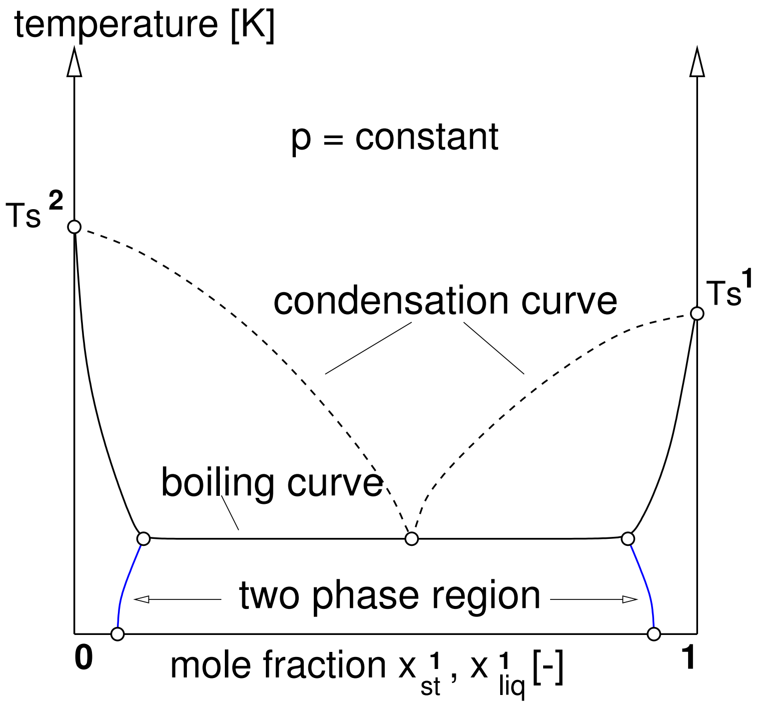
Water phase:

Henry's Law

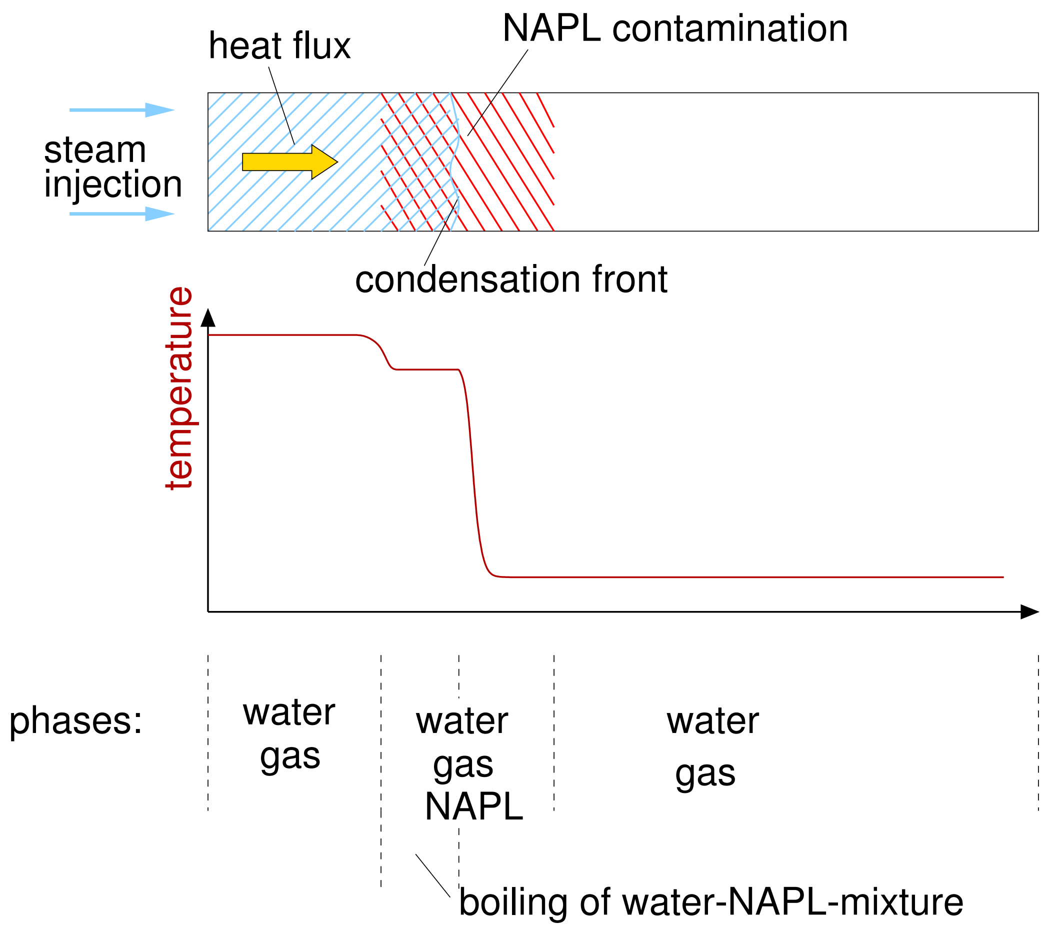
$$x_w^a = \frac{p_g^a}{H_w^a}, \qquad x_w^c = \frac{p_g^c}{H_w^c}$$

Boiling of a Water-NAPL Mixture

Boiling diagram, limited (low) miscibility



Characteristic temperature behavior during steam injection

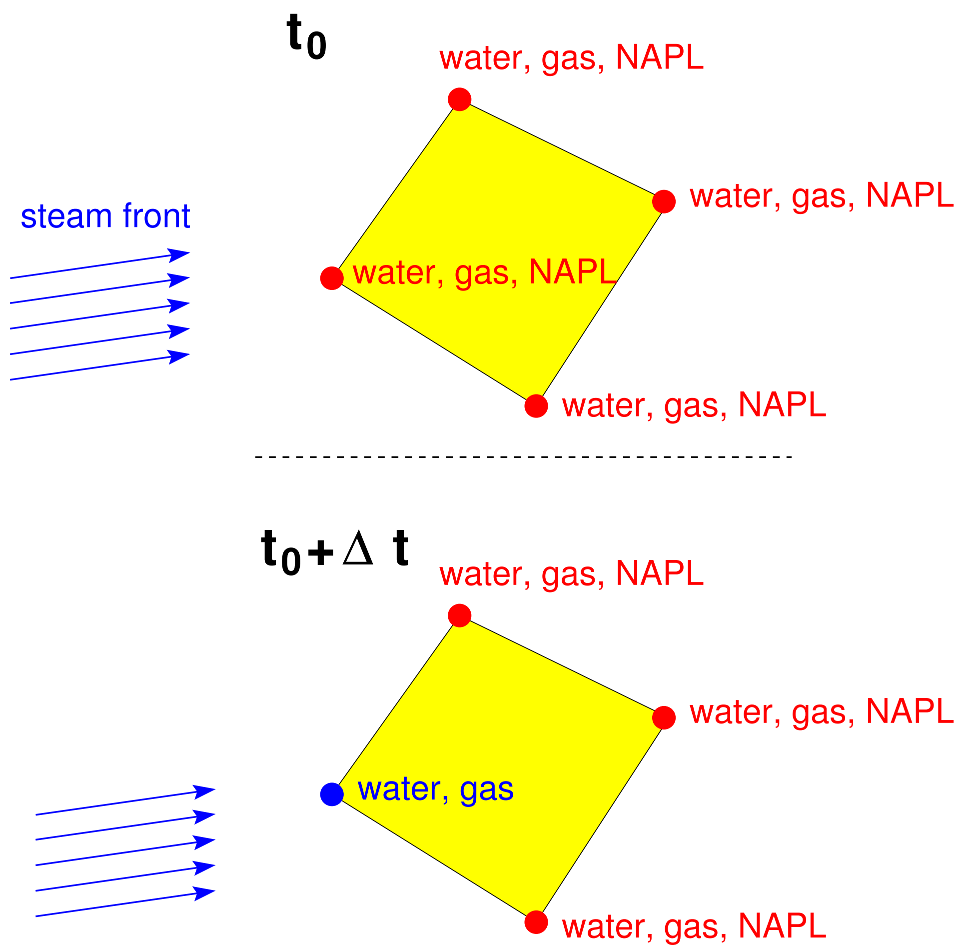


Adaptive Choice of Primary Variables

- Primary variables for determination of physical/thermodyn. state dependent on the *phase state*

phase state	primary variables
water, gas, NAPL	S_n, S_w, p_g, T
water	x_w^c, x_w^a, p_g, T
gas, NAPL	S_n, x_g^w, p_g, T
water, NAPL	S_n, x_w^a, p_g, T
gas	x_g^c, x_g^w, p_g, T
water, gas	x_g^c, S_w, p_g, T

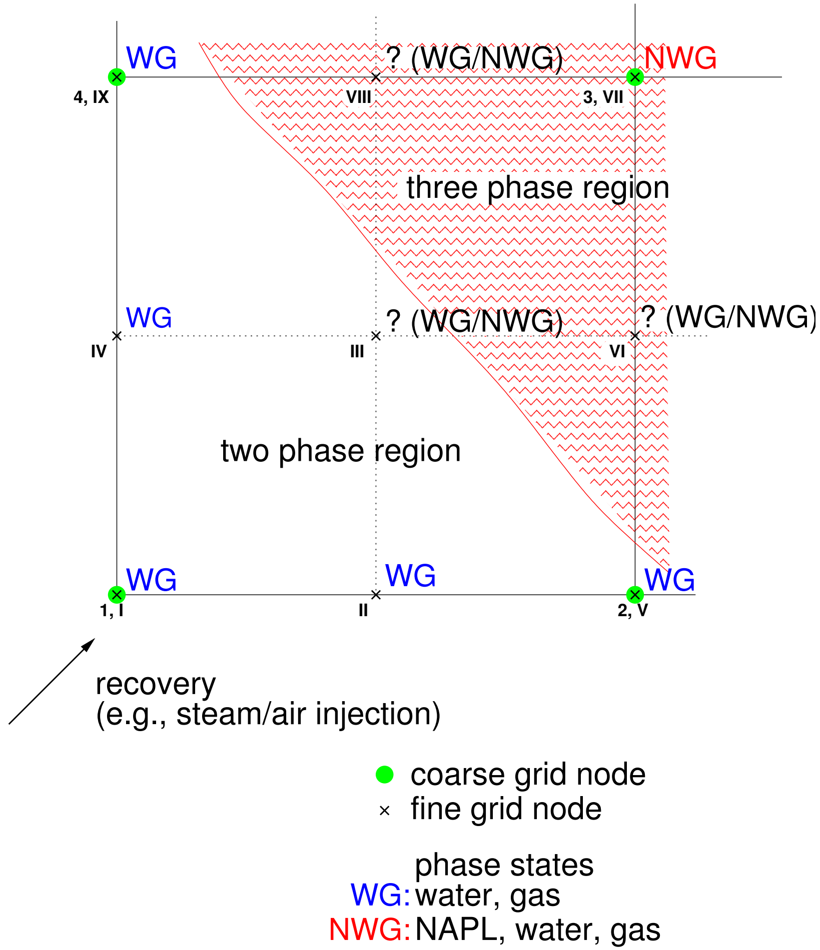
- Substitution criteria



Solution Methods

Coupled, nonlinear PDE
$\longrightarrow$ linearization (Newton-Raphson)

Solution of linearized equations
$\longrightarrow$ different options available in MUFTE_UG
e.g., direct solvers, BiCGStab, ILU, multigrid



Applying the multigrid method
for varying phase states

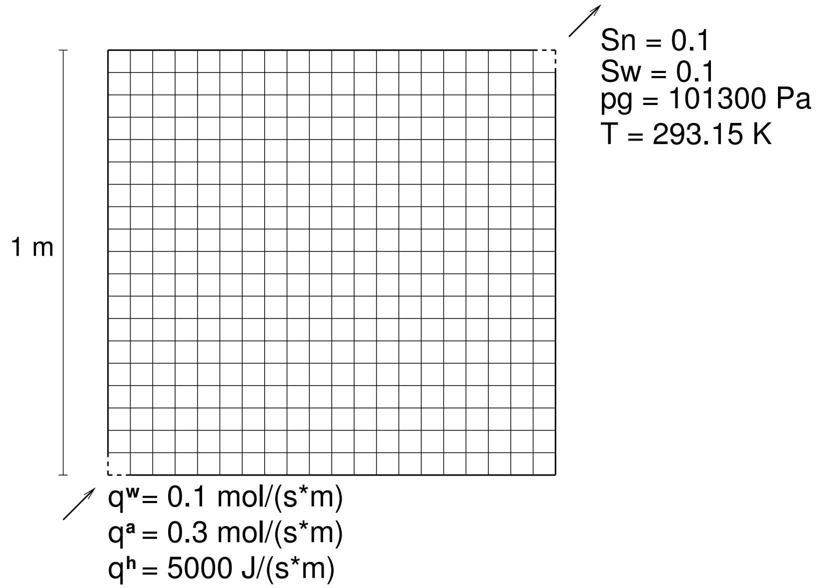
(Class, Helmig, Bastian, 2002)

Prolongation:

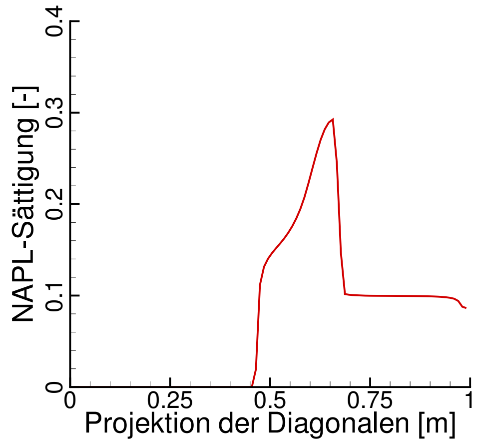
- Coarse grid corrections
  $\longrightarrow$ linear approximation
  $$e^i|_{x_k} = f_{x_k}(\mathbf{x}^i + \mathbf{e}^i) - f_{x_k}(\mathbf{x}^i)$$
- Phase states

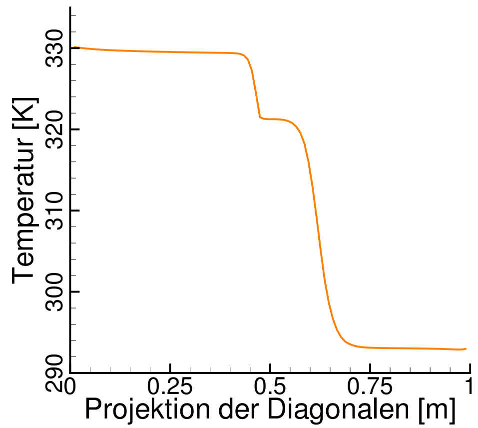
Application of the Multigrid Method

Coarse Grid: 400 elements



NAPL saturation und temperature after 3 hours:





- NAPL-contaminated domain
- Steam-air injection
- Change of phase state
  NWG $\longrightarrow$ WG

Application of the Multigrid Method

Different solution methods for the linearized problem:

1. Nested iteration, multigrid cycle (V) as preconditioner, BiCGStab on finest grid, direct solver on the coarse grid (desired optimum: convergence rate independent of grid size h)

2. Same as Case 1, but nested iteration only for computation of first time step

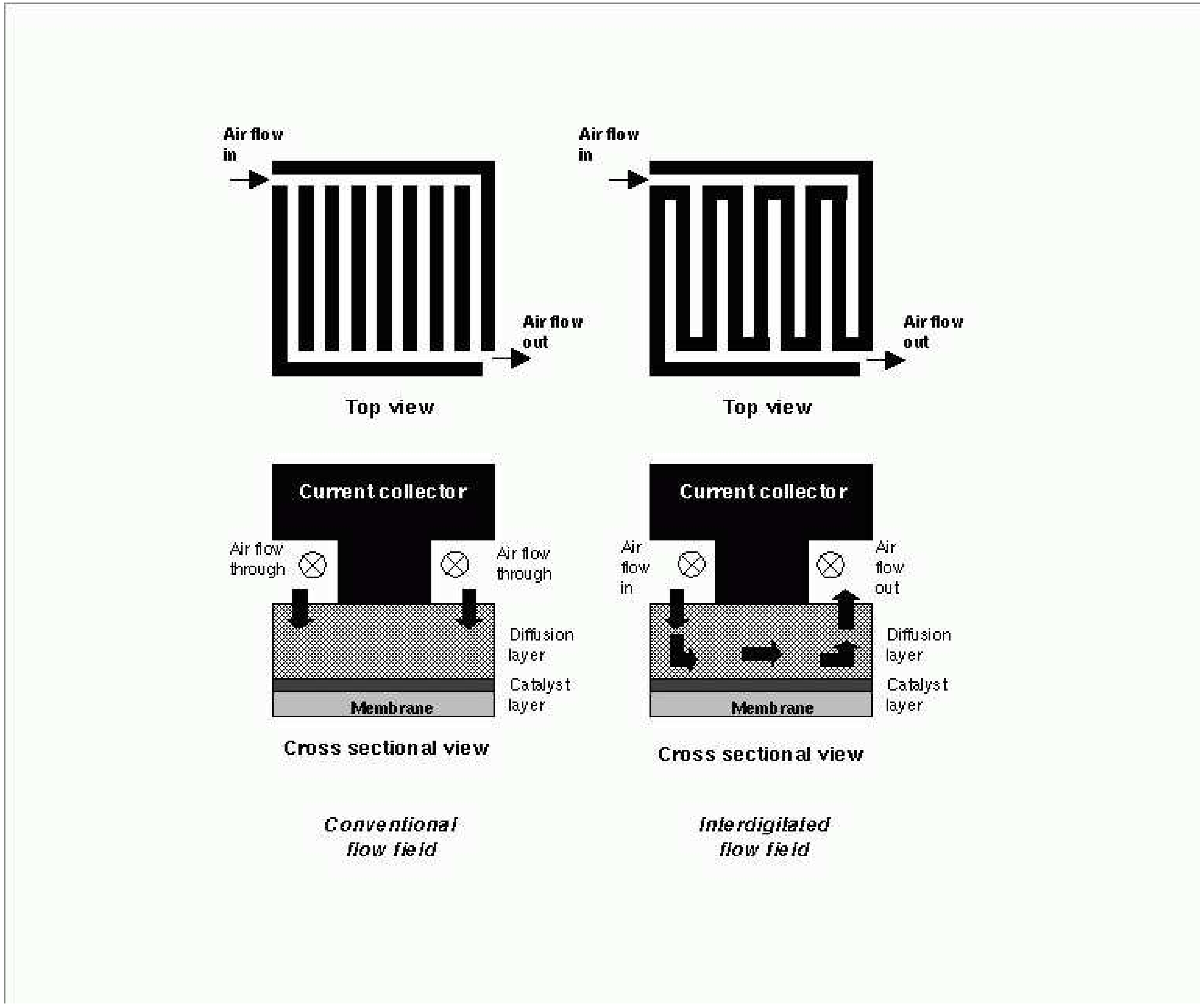
3. Same as Case 2, but ILU as preconditioner (expected convergence rate: $1 - \mathcal{O}(h)$)

(Class, Helmig, Bastian, 2002)

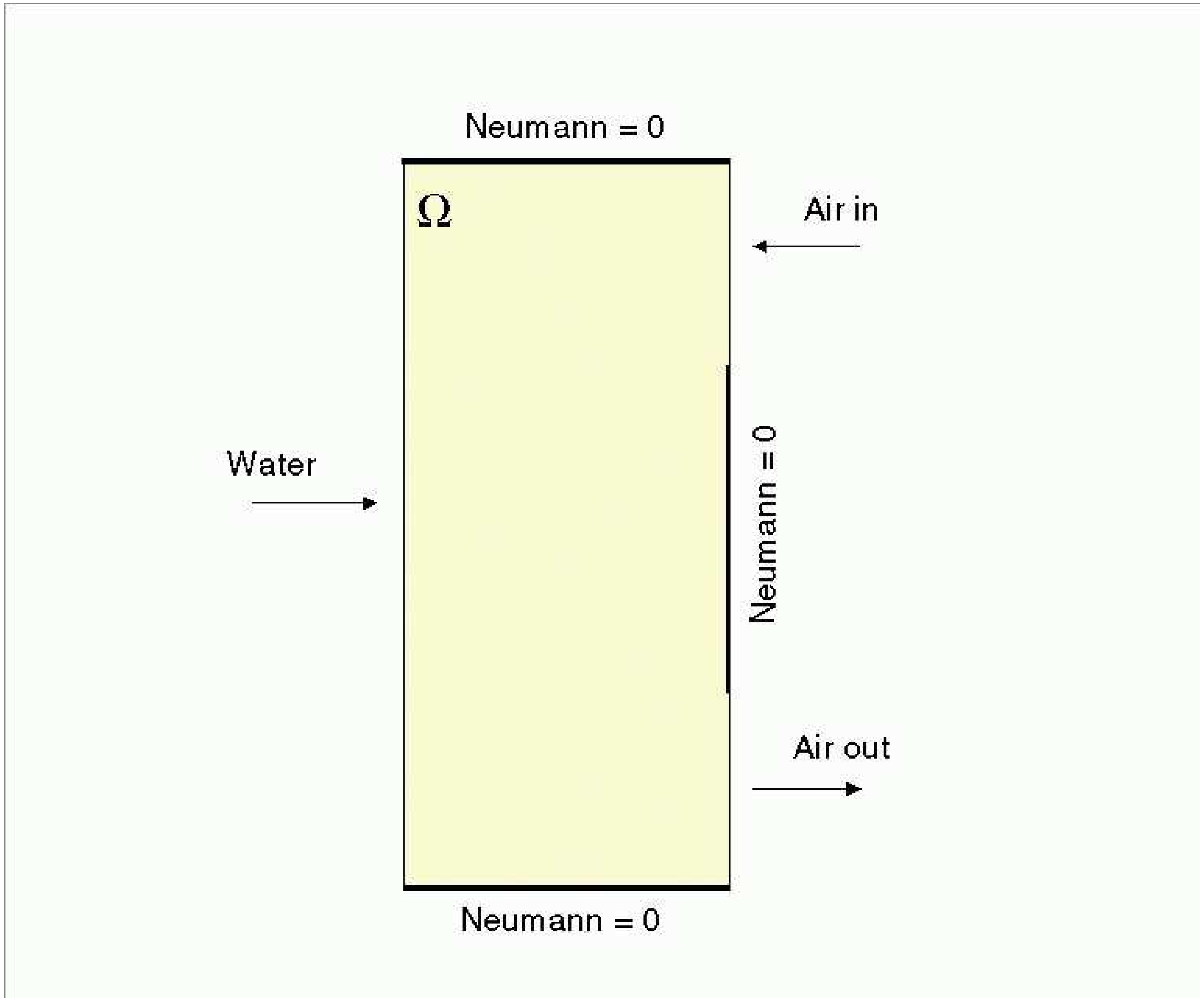
elements	exec. time	LIT/NLIT
SIMULATION PARAMETER CASE 1		
1600	7561	1.84
6400	$3.48 \cdot 10^4$	2.33
25600	$1.95 \cdot 10^5$	2.63
SIMULATION PARAMETER CASE 2		
1600	8126	3.04
6400	$6.28 \cdot 10^4$	3.94
25600	$5.16 \cdot 10^5$	4.12
SIMULATION PARAMETER CASE 3		
1600	8288	48.84
6400	$9.42 \cdot 10^4$	96.02
25600	$1.18 \cdot 10^6$	178.48

1600, 6400, 25600 elements
$=$ 1, 2, 3 refinement levels

Gas Current Collector



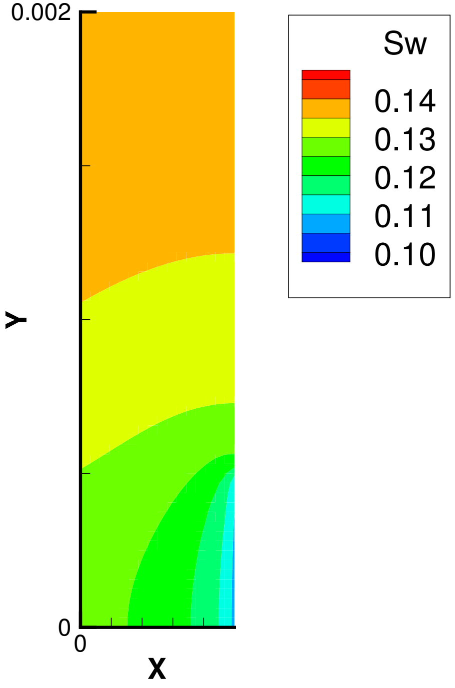
2D Model Domain



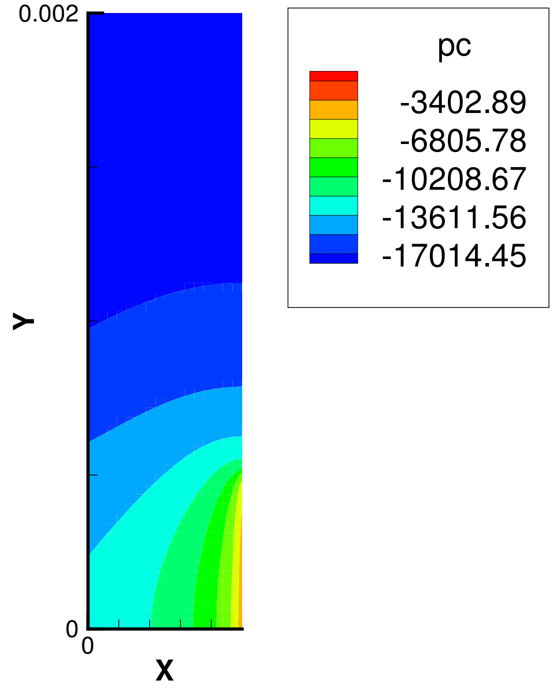
First simulations with MUFTE_UG

Steady-state:

water saturation



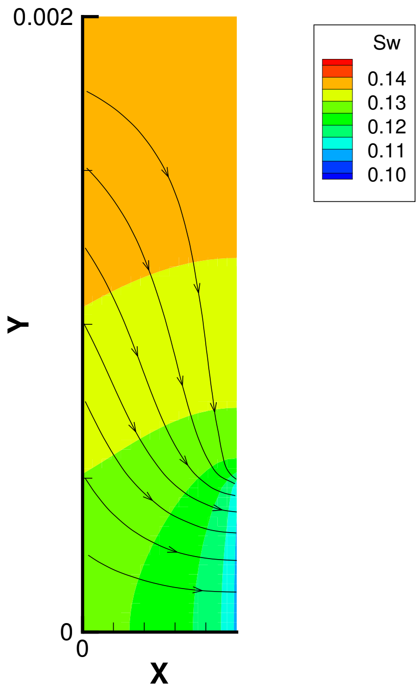
capillary pressure



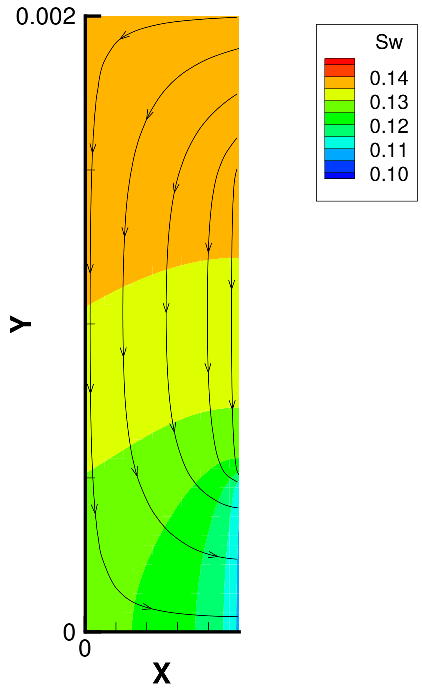
First simulations with MUFTE_UG

Flow directions:

water



gas



Final Remarks

- Examples show that numerical models are very important for the interpretation of strongly coupled processes.
- Fluid properties and thermodynamics are well known in the context of fluid-soil-properties.
- We need more information about the constitutive relationships for hydrophobic porous media (scale-dependent).
- Uncertainties arise from the interaction of the fluids with the porous media, e.g. phase dispersion, hysteresis.