Primary Variables
Variable Switching
Initial Conditions
Boundary Conditions

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General Concept

- Primary variables *completely* define the system state
- Choice of primary variables defines the phase state (single-phase vs. two-phase conditions)
- Initial conditions are the set of primary variables at the beginning of a simulation
- Dirichlet boundary conditions are given as *initial conditions* for inactive elements (or elements with a very large volume)
- The system state at the end of a simulation (stored on file *SAVE*) can be used as the initial conditions (file *INCON*) for a subsequent simulation

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Primary Variables – Secondary Parameters

- Assuming *local thermodynamic equilibrium*, the system state is defined by the number of balance equations per grid block, typically NK mass balance equations and one energy balance equation
- The primary variables are the time-dependent *unknowns* of the simulation, i.e., they are the *solution variables*
- The number of primary variables depends on EOS module (e.g., EOS9: 1; EOS3: 3; T2VOC: 4)
- Secondary parameters are fluid and state-related *properties* calculated as a function of the system state, i.e., sec. par. = *f*(prim. variables)

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Variable Switching

- Each element may be in a different phase state, i.e., may have a different set of primary variables
- Phase state may change during simulation (phase appearance/disappearance) → variable switching
- Primary variables are identified by their *position and value* (sometimes enhanced by a constant value, typically 10)
- *First* primary variable is (gas) *pressure*;
  Exception: EOS9 unsaturated
- *Last* primary variable is always temperature (even if isothermal conditions are chosen)
  Exception: EOS2, EOS4, EOS9

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Single-Phase vs. Two-Phase Conditions for EOS3 (1 of 3)

- (Second) primary variable for *single-phase* conditions is air-mass fraction in phase β, X_β^{air}
- (Second) primary variable for *two-phase* conditions is saturation $S_g + 10$
- 10 is added to S_g to distinguish between single- and two-phase conditions based on the numerical value alone:

  $0 \le X_\beta^a \le 1$ and $0 + 10 < S_g + 10 < 1 + 10$
- What is β in X_β^{air}, *l* (liquid) or *g* (gas)?
- How can we distinguish between single-phase *liquid* and single-phase *gas*?

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Single-Phase vs. Two-Phase Conditions (2 of 3)

- *Single-phase liquid*: $\boxed{0 \le X_\beta^a = X_l^{air} < X_{l,eq}^{air}}$
  - Value of X_β^{air} typically close to zero
  - Represents amount of air dissolved in liquid phase
  - Solubility limit $X_{l,eq}^{air}$ given by *Henry's law*
  - Typical value (P = 1 bar, T = 20°C): $X_{l,eq}^{air} \approx 1.6 \times 10^{-5}$
- *Single-phase gas*: $\boxed{X_{g,eq}^{air} < X_\beta^a = X_g^{air} \le 1}$
  - Value of X_β^{air} typically close to one
  - Represents amount of air present in gas phase
  - $X_{g,eq}^{air} = 1 - X_{g,eq}^{w}$ given by *vapor pressure curve*
  - Typical value (P = 1 bar, T = 20°C): $X_{g,eq}^{air} \approx 0.985$
- *Two-phase*: $\boxed{X_l^{air} = X_{l,eq}^{air} \text{ and } X_g^{air} = X_{g,eq}^{air}}$
  - X_β^{air} at equilibrium values determined by P and T
  - X_β^{air} no longer a prim. variable → initialize as $S_g + 10$

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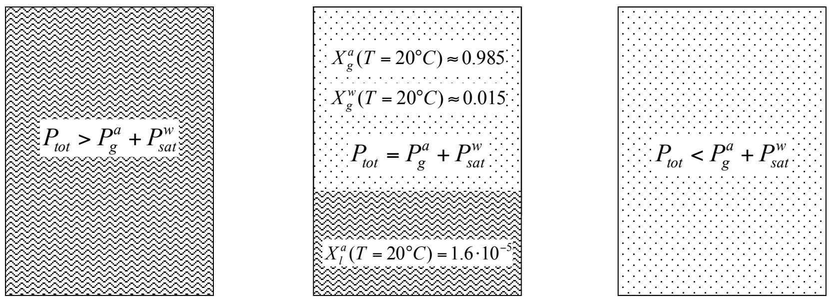
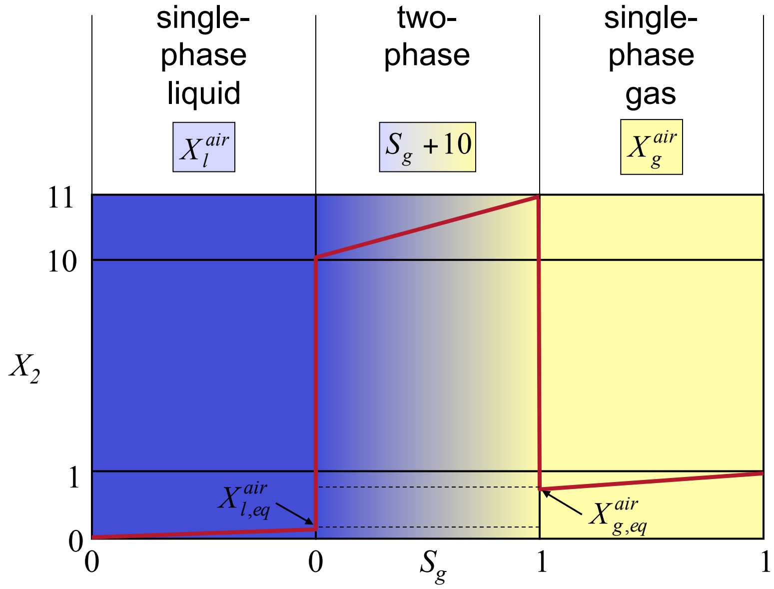
Single-Phase vs. Two-Phase Conditions (3 of 3)

Mass fraction: $X_\beta^\kappa = \dfrac{m_\beta^\kappa}{m_\beta} = \dfrac{m_\beta^\kappa}{\sum_{\kappa=1}^{NK} m_\beta^\kappa} = \dfrac{x_\beta^\kappa M^\kappa}{\sum_{\kappa=1}^{NK} x_\beta^\kappa M^\kappa}$ $\qquad \sum_{\kappa=1}^{NK} X_\beta^\kappa = 1 \qquad M^\kappa = m^\kappa / n$



Single-phase liquid P_g, X_l^a, T | Two-phase gas-liquid P_g, $10+S_g$, T | Single-phase gas P_g, X_g^a, T

Variable Switching



Specifying Initial Conditions

- Provide *default* initial conditions in block `PARAM.4`:
  - Apply to all elements
- Provide *domain-specific* initial conditions in block `INDOM`
  - Provide domain name from `ROCKS` and primary variables
  - Overwrites default values given through `PARAM.4`
- Provide *element-specific* initial conditions in block `INCON`
  - Provide element name and primary variables
  - Overwrites default and domain specific primary variables
- Provide keyword `START` if `INCON` does *not* provide initial conditions for *all* elements in *same order* as block `ELEME`
- File *SAVE* contains `INCON` block to be used for follow-up run
- Block `INCON` may be provided on external file *INCON*

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Dirichlet Boundary Conditions

- Constant pressure/saturation/temperature boundary conditions are specified as *initial conditions*
- To keep them constant, do one of the following:
  - Set the corresponding boundary element *volume* to a *very large* value (typically 1.0E50). The very large volume ensures that the system state in this element remains constant despite inflow/outflow of fluids and energy
  - Make boundary elements *inactive* by moving them to the end of block `ELEME`, *after* an element of *zero* or *negative volume*
- Specify constant temperature boundary conditions (but variable pressure/saturation) by setting rock *grain density* to a very large value (typically 1.0E50)

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Neumann Boundary Conditions

- Specified flow (Neumann) boundary conditions are specified through block `GENER`
- Neumann boundary conditions can be *constant* or *time-dependent* (tabular input)
- *Injection is positive, production is negative*
- For injection, specify mass flow rate of *component* κ (*not* phase β) and enthalpy
- For production, specify *total mass* of produced fluid mixture
- *Phase composition* for production is determined by phase composition and mobility of producing element (see also `MOP(9)`)

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Atmospheric Boundary (1 of 5)

- No atmospheric boundary element needed for Richards equation (EOS9)
- Specify Dirichlet boundary condition at land surface (i.e., inactive element or element with large volume; special rock type, e.g., `ATMOS`)
- A single atmospheric element can be connected to all elements at the ground surface (use, e.g., `AddBound.exe`)
- Use small nodal distance (e.g., boundary layer thickness) from atmospheric element to interface with first row of soil elements

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Atmospheric Boundary (2 of 5)

- Initial condition in atmospheric element:
  - Atmospheric pressure and temperature
  - For 100% relative humidity, use two-phase point with liquid saturation smaller than residual liquid saturation (so relative permeability is zero, preventing liquid flow into soil)
  - For less than 100% relative humidity, use single-phase gas point with appropriate air mass fraction X^a_g ($X^a_g=1.0$ for dry air; minimum value $X^a_{g,min}=1-X^w_{g,eq}$ depends on vapor pressure (which is a function of temperature); intermediate values $X^a_{g,min}(T) < X^a_g \leq 1.0$ determine relative humidity)

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Atmospheric Boundary (3 of 5)

- Material Properties for Atmosphere
  - Select relative permeability and capillary pressure functions so that (for the saturation given in the atmospheric boundary element):
    - Liquid relative permeability is *zero* at specified saturation
    - Gas relative permeability is *one* at specified saturation
    - Capillary pressure is *zero* at specified saturation
    - Ensure *upstream weighting* of mobilities (see `MOP(11)`)
- Infiltration
  - Specify infiltration rates in row of elements *below* the atmospheric boundary element using the `GENER` block
- Evaporation
  - Simulate as *binary diffusion* process (atmosphere at <100% r.h.)
  - Specify ET rate in row of elements *below* the atmospheric boundary element using the `GENER` block
  - Assign capillary pressure according to *Kelvin's equation* in atmospheric element (see Ghezzehei et al., *Vadose Zone J.*, 3: 806–818, 2004)

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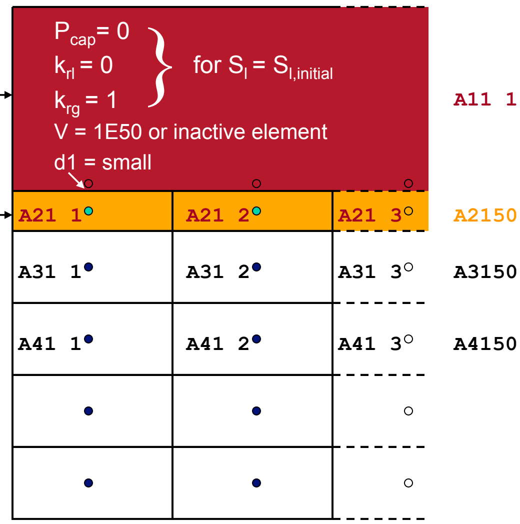
Atmospheric Boundary (4 of 5)

Dirichlet atmospheric b.c.:
Two-phase for 100% r. h.
$S_{l,initial} = 0.01 < S_{lr}$
Single-phase gas for < 100% r.h.
$X^a_{g,min}(T) < X^a_g \leq 1.0$

Neumann b.c.:
GENER, with rates
positive for infiltration and
negative for ET



Atmospheric Boundary (5 of 5)

```
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ATMOS    2     2650.     .9999                     1.000E-12      2.51   100000.
                                     1.0
    1            0.1       0.0       1.0       0.1
    1            0.0       0.0       1.0
SOIL     0     2650.     .3000 1.000E-12 1.000E-12 1.000E-12      2.51      920.

ELEME
A11 1          ATMOS0.1000E+510.1000E+01                                     0.0
A21 1          SOIL 0.5000E-010.0000E+00          0.5000E+000.5000E+00-.2500E-01
A31 1          SOIL 0.5000E-010.0000E+00          0.5000E+000.5000E+00-.7500E-01
.....              .....................          ..............................
A2150          SOIL 0.5000E-010.0000E+00          0.1000E+010.5000E+00-.2500E-01
A3150          SOIL 0.5000E-010.0000E+00          0.1500E+010.5000E+00-.7500E-01
..........                   .........................................

CONNE
A11 1A21 1                   30.5000E-020.2500E-010.1000E+010.1000E+01
A11 1A21 2                   30.5000E-020.2500E-010.1000E+010.1000E+01
..........                   .........................................
A11 1A2150                   30.5000E-020.2500E-010.1000E+010.1000E+01
..........                   .........................................
A2250A3150                   30.2500E-010.2500E-010.1000E+010.1000E+01
..........                   .........................................

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1
             1.013E5               10.99                20.0

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A21 1INF 1   49    1    1          WATE     1.0E-4
```