Numerical modelling of high temperature geothermal systems with a soil-atmosphere boundary condition.

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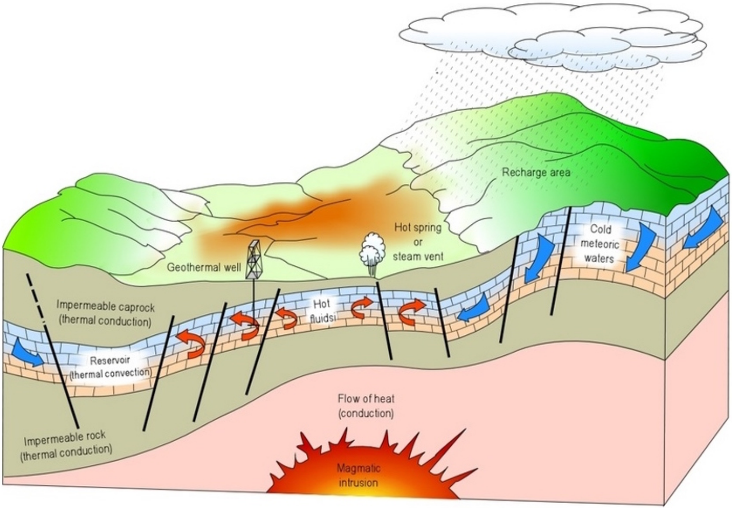
A high temperature geothermal system



Dickson & Fanelli 2015

Numerical simulation

Numerical simulation of the molar flows and the thermal transfers.

- Geothermal modelling
  - liquid and gas phase flows, several components (water, air, salt, ...),
  - no mechanic, no chemistry,
  - formulation (which equations, which principal unknowns).
- Some difficulties:
  - robust formulation (coupling between T and P, change of phase, high variations of densities),
  - general boundary conditions,
  - general meshes (topography, faults).

Layout

1. Non-isothermal compositional two-phase flows
   - Porous medium model
   - Formulation and discretization
2. Soil-atmosphere boundary condition
3. 2D geothermal simulations

Single phase Darcy flow

$$\begin{cases} \text{Darcy law:} & \mathbf{q} = -\frac{\boldsymbol{\Lambda}(\mathbf{x})}{\mu}\Big(\nabla P - \rho(P)\mathbf{g}\Big), \\ \text{molar conservation:} & \phi \partial_t \zeta(P) + \mathrm{div}(\zeta(P)\mathbf{q}) = 0. \end{cases}$$

P: pressure (Pa)

$\mathbf{q}$: Darcy velocity ($\mathrm{m.\,s}^{-1}$)

$\boldsymbol{\Lambda}(\mathbf{x})$:permeability tensor of the porous medium (m^2)

ϕ: porosity of the porous medium

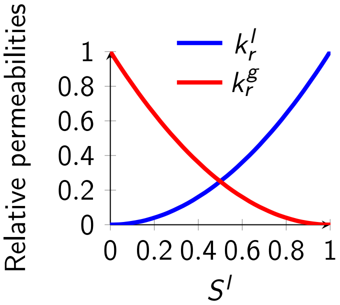
μ: viscosity of the fluid ($\mathrm{Pa.\,s}$)

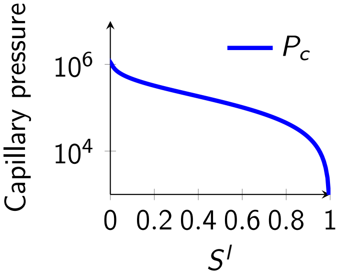
ζ: molar density of the fluid ($\mathrm{mol.\,m}^{-3}$)

ρ: mass density of the fluid ($\mathrm{kg.\,m}^{-3}$)

Two phase Darcy velocities

$$\begin{cases} \mathbf{q}^\alpha = -\frac{k_r^\alpha(S^\alpha)}{\mu^\alpha}\mathbf{\Lambda}(\mathbf{x})\Big(\nabla P^\alpha - \rho^\alpha \mathbf{g}\Big), \\ P^g - P^l = P_c(S^g), \\ S^g + S^l = 1. \end{cases}$$





$\alpha = g, l$: phases
S^α: volume fractions
P^α: pressures
P_c: capillary pressure (in Pa)

Non-isothermal compositional liquid-gas Darcy equations

Molar conservation of each component $i \in \mathcal{C}$, typically $\mathcal{C} = \{\text{water}, \text{air}\}$

$$\phi \partial_t n_i + \operatorname{div}\Big(\sum_{\alpha = g, l} \zeta^\alpha c_i^\alpha \mathbf{q}^\alpha \Big) = 0, \quad i \in \mathcal{C},$$

together with the energy conservation

$$\partial_t \Big(\phi \sum_{\alpha = g, l} \zeta^\alpha e^\alpha S^\alpha + (1 - \phi) e_r \Big) + \operatorname{div}\Big(\sum_{\alpha = g, l} \zeta^\alpha h^\alpha \mathbf{q}^\alpha \Big) + \operatorname{div}(-\lambda \nabla T) = 0$$

complemented by local closure laws $P^g - P^l = P_c(S^g)$ and $S^g + S^l = 1$ and the **thermodynamic equilibrium**.

$c^\alpha = (c_i^\alpha)_{i \in \mathcal{C}}$: molar fractions
$n_i = \sum_{\alpha \in \mathcal{P}} \zeta^\alpha \; S^\alpha \; c_i^\alpha$: number of moles per unit pore volume
e^α: molar internal energy, $\quad h^\alpha$: molar enthalpy, $\quad \lambda$: thermal conductivity

Two families of formulations

- **Variable switch formulations**
  - Coats' formulation[1]: $U^{Coats} = \left(\mathcal{Q}, P^g, P^l, T, S^g, S^l, C^\alpha, \alpha \in \mathcal{Q}\right)$ where $\mathcal{Q}$ is the set of present phase(s).

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[1] Coats 1989.

[2] adapted from PSF formulation (isothermal case) in A. Lauser et al 2011.

[3] I. Ben Gharbia and J. Jaffré 2014.

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    where $\mathcal{Q}$ is the set of present phase(s).

- **Persistent variable formulations**
  - T-PSC[2]: $U^{PSC} = \left(P^\alpha, T, S^\alpha, \bar{C}^\alpha, \alpha \in \mathcal{C}\right)$,

  No switch of variables: **extension of the phase molar fractions** $\bar{C}^\alpha$.
  Thermodynamic equilibrium: **complementarity constraints**

$$S^\alpha \geq 0, \quad 1 - \sum_{i \in \mathcal{C}} \bar{C}_i^\alpha \geq 0, \quad S^\alpha (1 - \sum_{i \in \mathcal{C}} \bar{C}_i^\alpha) = 0, \qquad \alpha = g, l,$$
$$f^g(P^g, T, \bar{C}^g) = f^l(P^l, T, \bar{C}^l).$$

  which allows the use of **semi-smooth Newton methods**[3].

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Discretization

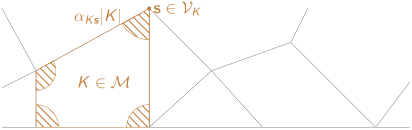
- Fully implicit Euler scheme
- Finite volume in space: **Vertex Approximate Gradient**[4]
- Phase based upwind scheme for the approximation of the mobilities, molar fractions and enthalpies
- Newton-min non-linear solver (thanks to the complementarity constraints)

Splitting between $\#\mathcal{C} + 1$ primary unknowns + the remaining secondary unknowns.

[4] Eymard et al 2010.

Vertex Approximate Gradient (VAG)

- Allow unstructured meshes
- Nodal based scheme (cell unknowns are eliminated without fill-in): cheap on tetrahedral meshes
- Control volume scheme: mass or energy balance equation for each non Dirichlet degree of freedom



Remark 1: if cellwise constant rocktypes in the matrix, it is sufficient to define the matrix volume fractions.

Remark 2: flexibility in the choice of the control volumes (important at the boundary between different rocktypes, or fractures).

Newton-min non-linear solver

- **Basic version**: enforces only $P^g - P^l = P_c(S^g)$, needs the projection $C^\alpha \in [-0.2; 1.2]$.
- **Newton-min with projection on the complementarity constraints**:

$$\text{previous updates} + \begin{cases} \min(U_1, U_2) = 0, \\ \text{if } S^\alpha > 0 \text{ then } 0 \leq C^\alpha \leq 1, \quad \alpha = g, l, \\ \sum_{\alpha=g,l} S^\alpha = 1 \text{ and } 0 \leq S^\alpha. \end{cases}$$

Additional: test the appearance of α using non-linear updates of C^α.

- **Newton-min with projection on the complementarity constraints and thermodynamic equilibrium**: previous updates +

$$\left.\begin{array}{l} C^\alpha \text{ (which are 2}^{\text{nd}} \text{ unknowns)} \\ T \text{ (if both phases are present)} \end{array}\right\} \text{are updated to verify } f^g = f^l.$$

Layout

Why a soil-atmosphere boundary condition?

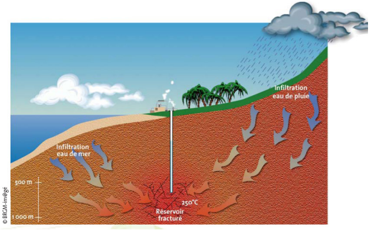


Figure: Sketch of a main fault of Bouillante.

High temperature close to the surface

- 250 °C at -300m
- approaches 100 °C at the surface

But the coupling

(porous medium + surface flows)

is **not computationally realistic**.

Objective:

soil-atmosphere boundary condition

BC: vaporization and liquid outflow

BC based on **mole and energy balance equations set at the interface**. Far field atmospheric conditions $C_\infty^{g,atm}$, T_∞^{atm}, P^{atm} are imposed.

Additional unknowns:

$q^{g,atm}$ (gas molar flow rate), $q^{l,atm}$ (liquid molar flow rate).

Two modes (automatic transition between them):

- **assuming instantaneous vaporization of the liquid phase**
  $\rightarrow$ convective molar and energy transfer (of coef. H_m and H_T), with:
  - continuity of the component molar and energy normal fluxes,
  - continuity of the gas phase (C^g, T, P^g).
- **vaporization + liquid outflow**.

Fluxes balance at the interface

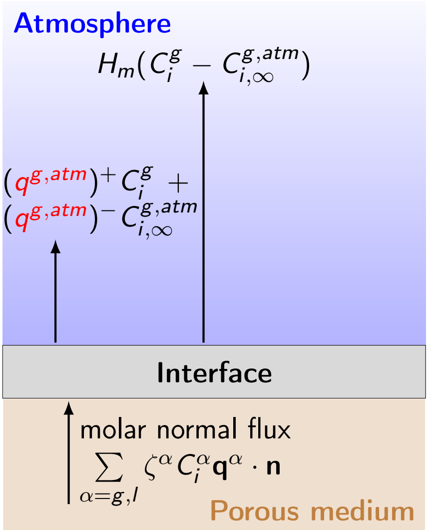


Figure: Molar fluxes balance.

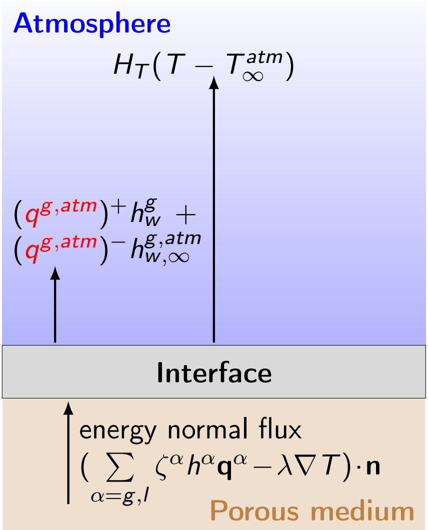
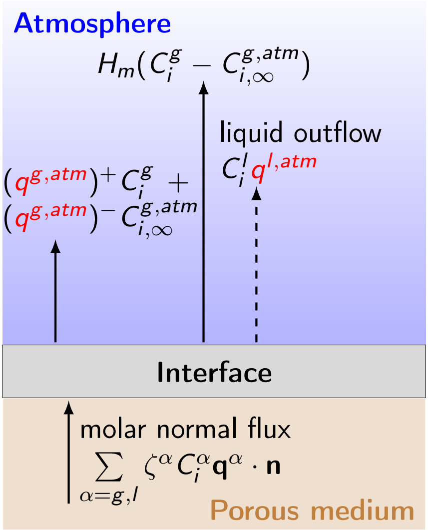


Figure: Energy fluxes balance.

Fluxes balance at the interface



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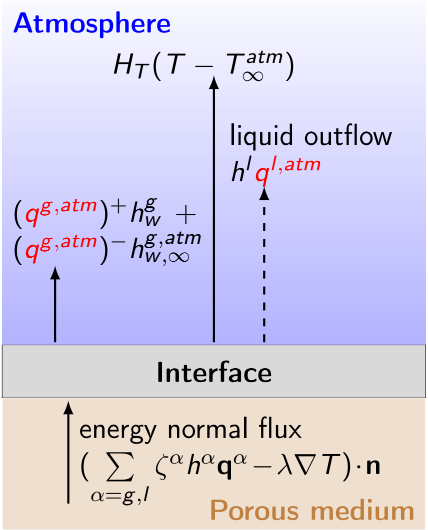

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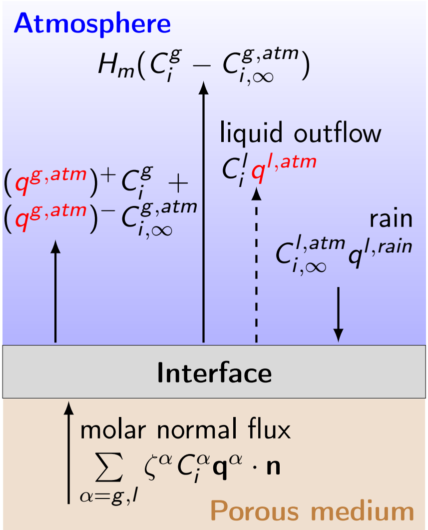

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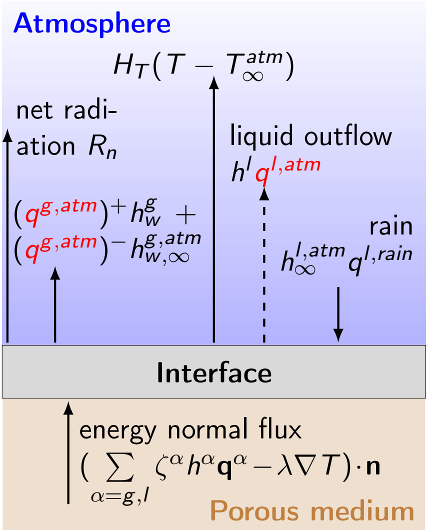


Figure: Energy fluxes balance.

Transition to vaporization + liquid outflow

At the interface:

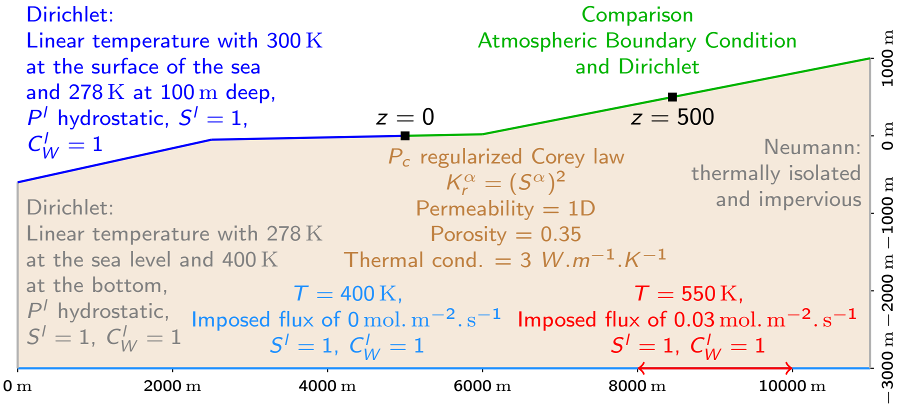
$$\begin{cases} \text{on the atmosphere side: } \min\left(q^{l,atm}, 1 - \sum_{i \in \mathcal{C}} C_i^{l,atm}\right) = 0, \\ \textbf{thermodynamic equilibrium}, \\ \textbf{continuity of the gas phase}, \end{cases}$$

gives

$$\boxed{\min\left(q^{l,atm}, P^g - P^l\right) = 0.}$$

Layout

2D main fault of Bouillante



Liquid density and viscosity are fixed to prevent thermal instabilities.

BC at the upper boundary ($0 < z$)

Soil-atmosphere BC:

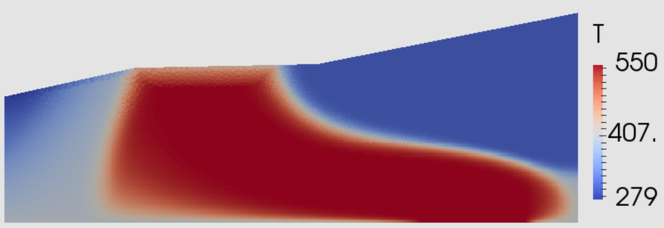
- $C_\infty^{g,atm}$, T_∞^{atm}, P^{atm}, far field atmospheric conditions with $Hur = 0.5$,
- $(1-a)R_s + R_a = 340\ W/m^2$, $\epsilon = 0.97$, $H_m = 0.69\ mol/m^2/s$, $H_T = 29 * H_m = 20\ W/m^2/K$[5],
- Precipitation recharge ($500 < z$): $q^{l,rain} = -0.032\ mol/m^2/s$, $C_{w,\infty}^{l,atm} = 0.999$ (twice the observed rainfall in 2016).

Dirichlet BC:

- Sunny plain ($0 < z \leq 500$) far field atmospheric conditions: $S^g = 1$, $C^g = C_\infty^{g,atm}$, $P^g = P^{atm}$, $T = T_\infty^{atm}$,
- Rainy zone ($500 < z$) deduced from Atmospheric BC: $S^g = 0.72$, $C_a^g = 0.97$, $C_w^l = 0.999$, $P^g = 1\ atm$, $T = 300\ K$.

[5] from Monteith and Unsworth 1990.

Temperature with the soil-atm BC



Temperature and gas saturation above the threshold of 10^{-2}

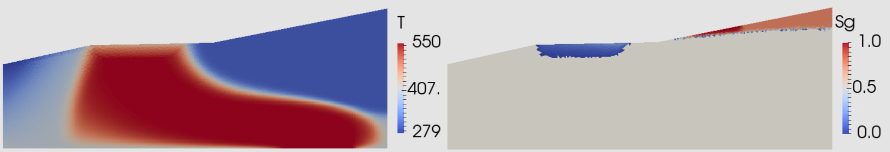


Figure: Atmospheric boundary condition.

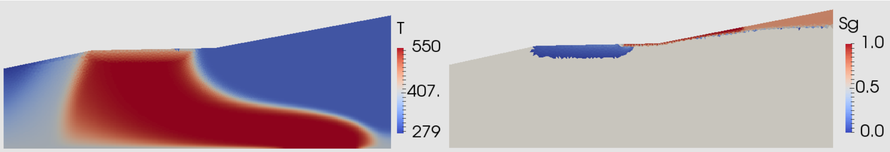


Figure: Dirichlet boundary condition.

Temperature and gas saturation above the threshold of 10^{-2}

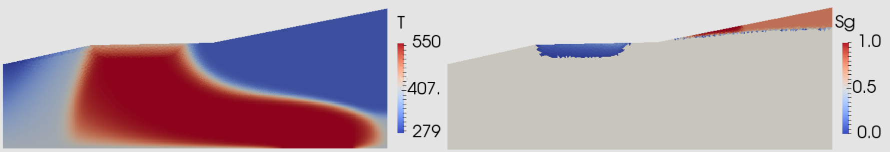


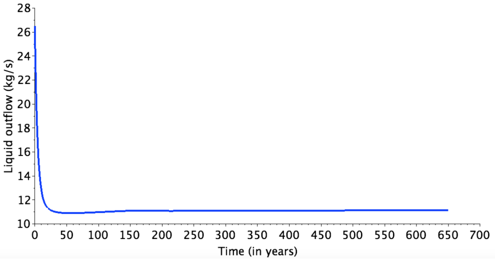
Figure: Atmospheric boundary condition.

Liquid outflow:

$$\min\left(q^{l,atm}, P^g - P^l\right) = 0,$$

with

$$P_c(0) = 0.$$



Conclusions and Perspectives

Formulation and model of a soil-atmosphere BC:

- captures the evaporation and if necessary the liquid outflow,
- has a non-negligible impact on the geothermal simulation,
- is easier to set than Dirichlet constants.

TODO: more complex geometries and geologies, 3D with the ComPASS code (new geothermal simulator with unstructured meshes, adapted to parallel distributed architectures with the ability to represent fractures):

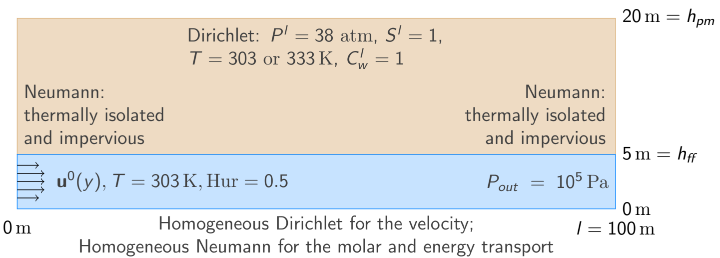
- adapt to Coats,
- pb of convergence of the linear and non-linear solvers,
- interaction with fractures ?

Thank you for your attention

Comparison to a full-dimensional free-flow model

Non-isothermal compositional Reynolds Average Navier-Stokes (RANS) gas flow, with at the interface

- vaporization of the liquid phase in the free-flow domain,
- continuity of the gas molar fraction,
- continuity of the molar and energy normal fluxes,
- liquid gas thermodynamic equilibrium,
- no slip condition,
- continuity of the normal component of the normal stress.



$T^0_{pm} = 303\ \mathrm{K}$ in the porous medium

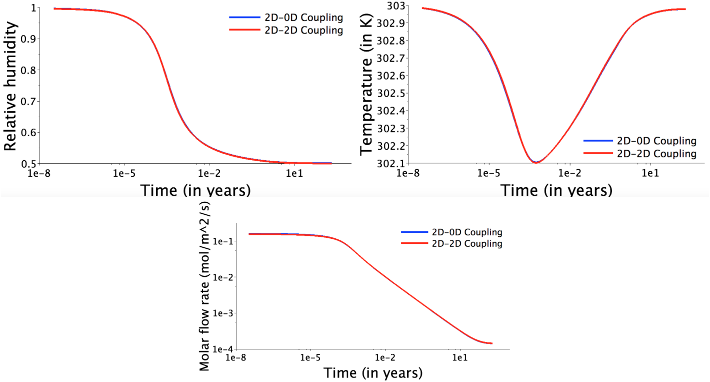


Figure: Values at the interface with $T^0_{pm} = 303\,\mathrm{K}$.

$T_{pm}^0 = 333\ \mathrm{K}$ in the porous medium

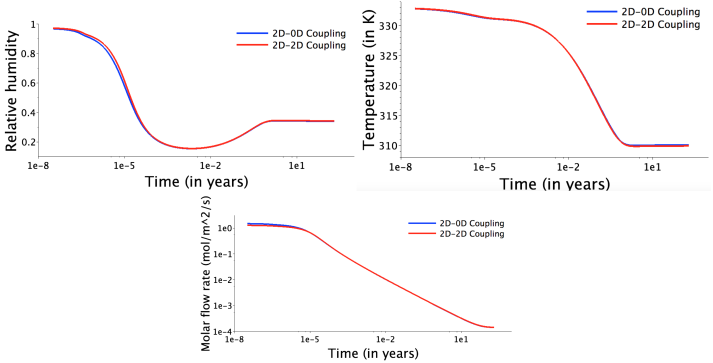


Figure: Values at the interface with $T_{pm}^0 = 333\,\mathrm{K}$.