Action d'envergure C2S@Exa
The Traces software

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Summary

1. Traces historic
2. Hydraulic and transport models
3. Numerical methods
4. Needs

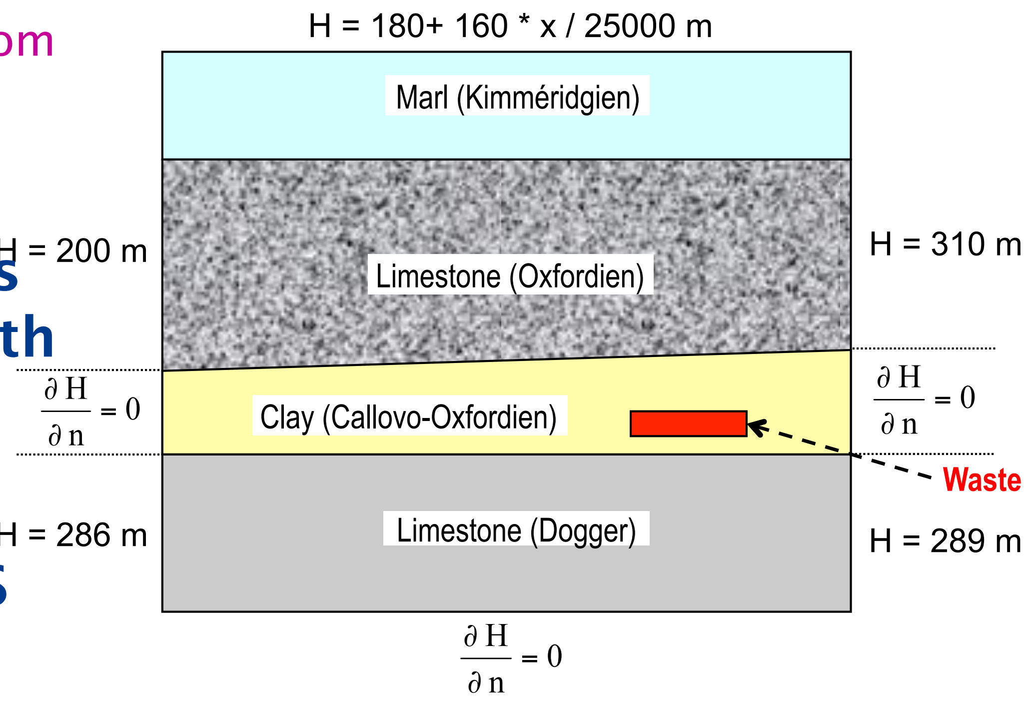
Traces historic

Transport RéActif de Contaminant dans les Eaux Souterraines
Transport of RadioACtive Elements in Subsurface

2001

Once upon a time, the Couplex exercise

- Compute a simplified Far Field model used in numerical waste management simulations
  - Convection diffusion type problem
  - Huge parameter variation from one layer to another



The IMFS laboratory gave a excellent numerical analysis and the obtained results with Traces code were "good"

It's the beginning of a partnership between IMFS and Andra

1.2 Traces evolutions (I)

2002-2003

Traces code is integrated in Andra platform as numerical component for :

- ☐ Saturated Hydraulic and transport module
- ☐ Reactive transport module

Main difficulty: the transport CPU time is too large when the problem is convective

- ☐ Explicit time discretization (EFD)

2004-2005

Development of implicit time discretization scheme for EFHM

Integration of new solver libraries : NSPCG, SLAP

Traces code is used to confirm the safety assessment results

1.2 Traces evolutions (II)

2006-2007

Development of the unsaturated hydraulic and transport model (Richards approximation)

2007-2009

Traces is used as transport code in a thesis about the identification of the geological layers and the associated transport parameters

- ☐ Inverse problem by adjoint-state method
- ☐ Automatic differentiation of code Traces with Tapenade Software

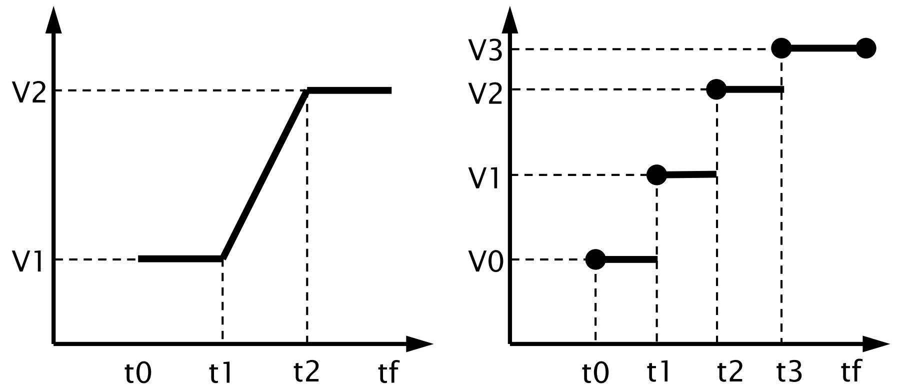
Development of the unsaturated hydraulic and transport model (Richards approximation)

IMFS: thesis of M. FAHS (2007) and C.P. EL SOUEDY (2008)

2010-2013

Parameters and boundary conditions can be defined as function of space and/or time

- Values by cells
- Linear or discrete interpolation



In transport calculation, flow (Darcy velocity and saturation) can be read from another calculation results

- Linear or discrete Flow (Darcy and saturation) interpolation
- Chaining two-phase flow and Kd-Csat transport calculation
- Use of specific time discretization for each physical phenomena

Hydraulic and transport models

Hydraulic

- Darcy law $\vec{U} = -\overline{\overline{K}}.\vec{\nabla}h$
- Mass conservation $div\left(\overline{\overline{K}}.\vec{\nabla}h\right) + s = 0$

Transport

- Mass conservation

$$\frac{\partial\left(R\phi_e.C_i\right)}{\partial t} = div\left(\overline{\overline{D_i^*}}.\vec{\nabla}C_i - C_i.\vec{U}\right) - \lambda_i.\phi_e.R_i.C_i + \sum_{j\in I}\sigma_{ij}\lambda_j.\phi_e.R_j.C_j + \phi_e.S_i + Q_i$$

+ Sorption
+ Diffusion-dispersion-convection
+ Decay, chain
+ Precipitation/dissolution

Parameter properties

- Anisotropy (full tensor)
- High contrast

2.2 Unsaturated porous media

Hypothesis

- No gas phase
- Constant viscosity and density
- No retroaction from hydraulic on transport

Hydraulic

- Mass conservation $\frac{\partial(\phi_e . S^l . \rho)}{\partial t} + div(\rho \vec{U}) = m$
- Darcy law $\vec{U} = -\frac{\overline{\overline{k}}.k_r}{\mu}.(\vec{\nabla} p + \rho . g . \vec{\nabla} z) = -\overline{\overline{K}}.\vec{\nabla} h$
- Permeability and saturation laws $\overline{\overline{K}} = \frac{\overline{\overline{k}}.k_r . \rho . g}{\mu}$ $k_r = k_r(\hat{S}^l)$ $\hat{S}^l = \hat{S}^l(\Psi)$ $\hat{S}^1 = \frac{S^1 - S_r}{1 - S_r}$
- Deformation of porous media $\phi_e = \phi_e(p)$ $\left(\frac{\partial \phi_e}{\partial p}\right) = \alpha_s$

Transport

- As in saturated porous media, but parameters depend from saturation

Numerical methods

3.1 Geometry and spatial discretization

Geometry

- Cartesian coordinates in 2D or 3D
- All types of elements :
  - triangle, quadrangle, tetrahedron, hexahedron, prism

Hydraulic discretization

- Mixed hybrid finite element method
  - + *Good Darcy velocity approximation*

Transport discretization

- Two possibilities:
  - Mixed hybrid finite element method
    - + *Facility to take into account the full tensors and mass balance on each element*
  - Mixed hybrid finite element method for dispersion and discontinuous Galerkin finite element method for convection
    - + *Accuracy, continuity of dispersive flaw*

3.2 Time discretization schemes, reactive process

Hydraulic

- Mixed hybrid finite element
  - First order Implicit scheme

Transport

- Mixed hybrid finite element
  - First order implicit scheme
- Mixed hybrid finite element and discontinuous Galerkin finite element
  - Time splitting operator
    - *First order implicit for dispersive and reactive part*
    - *Explicit for convective part*
      - Second order accurate based on explicit Runge-Kutta method
      - Stability is ensured by slope limiters
      - Necessity to respect the CFL criteria

Coupling with reactive process

- Linearization using the Picard method

First solveur

- PCG with Eisenstat procedure

Solvers added by Andra

- One direct solver: Gauss decomposition
- Solvers of NSPCG library
- Solvers of SLAP library

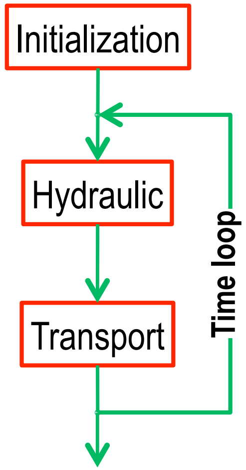
Needs

Calculation of elementary matrices

- Using programs generated with Maple procedure
  - These routines can't be modified or corrected
  - Interpolation isn't exact for cells whose the shape isn't regular
- It's also possible to use numerical integration

Hydraulic and transport problem

- Traces solves flow equations then, the transport equations
  - There is no iteration between hydraulic and transport calculation
  - Difficulties of convergence if the time step is too large
    - + *Unsaturated transport*
    - + *Reactive process*



4.2 Solver Performances (I)

Mixed hybrid finite element

- Large number of degrees of freedom
  - The solver performance is important
- Example 1: flow calculation
  - Regular mesh with **362 304** cells, 284 375 points, 1 110 680 faces
  - Number of degrees of freedom
    - *Porflow: 405 840*
    - *Traces: close to the number of faces*
  - CPU Times (minutes)

	NSPCG/CONJ/CHOL	NSPCG/CONJ/NEUM	NSPCG/GMRES/NEUM
Porflow	4	86	No convergence
Traces	15 (176 avec SLAP)	36	76

4.2 Solver performances (II)

- Example 2:
  - Regular mesh with **2 580 786** cells, 2644920 points, 7 806 021 faces
  - Hydraulic:
    - *Matrix: **7 738 593** degrees of freedom, **46 113 243** values*
    - *NSPCG/GMRES/NEUMANN did not converge in 20 000 iterations*
    - *NSPCG/CONJ/CHOL converge in 6675 iterations, cpu time: ≅7 hours*
    - *SLAP/CG/CHOL converge in 6014 iterations*
  - Transport:
    - *Matrix: **7 678 695** degrees of freedom*
    - *NSPCG/GMRES/NEUMANN: ≅18 hours for 460 time steps*

Currently, the same solver is used for flow and transport calculation

- Difficulty of convergence in coupled problem

4.3 Others

Coupled problem

- Use different solvers for hydraulic and transport
- Change time discretization when there are convergence difficulties (nonlinear process)

Input optimization

- Build the face (or edge) table in the Traces code itself
- Reduce the number of input files
  - Even for a flow calculation, the Transport input files are required

Outputs Optimization

- Reduce the number of zone output files (these files can be very large)