Simple and efficient TRANsport Simulation Environment for density-driven fluid flow and coupled transport of heat and chemical species

- Most available open-source simulators limited by tightly integrated chemical modules with insufficient capabilities
- General lack of flexible interfaces applicable for an efficient coupling of third-party chemical libraries
- Available open-source numerical frameworks generally too complex to teach geosciences students about critical handling of simulation results

- FDM implementation of coupled density-driven Darcy flow, heat and species transport with ~700 lines of easily readable Python code
- Explicit, semi-implicit and fully implicit solution of coupled equations
- Execution times in the same order of C/C++/FORTRAN codes (JIT compiler)
- Full flexibility when coupling (geo-)chemical modules

EGU General Assembly 2020

ERE6.1 Process quantification and modelling in subsurface utilisation | Thu, 07 May, 10:45–12:30

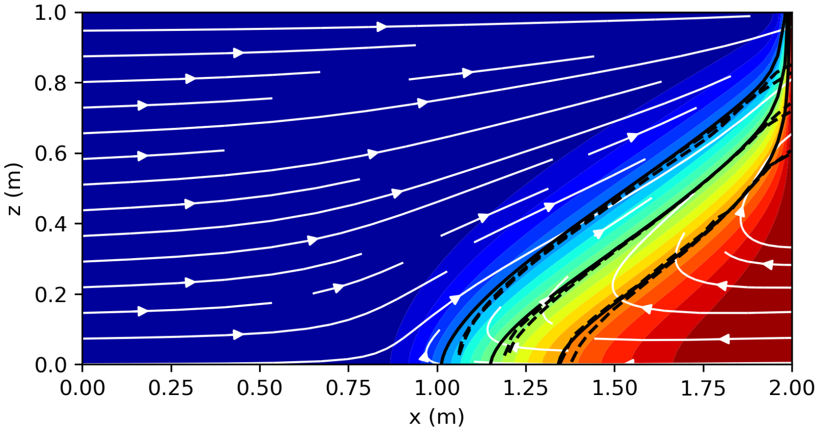
GFZ Helmholtz Centre Potsdam

Thomas Kempka[1,2]
[1]GFZ German Research Centre for Geosciences, Fluid Systems Modelling, Potsdam, Germany
[2]University of Potsdam, Institute of Geosciences, Germany
kempka@gfz-potsdam.de

HELMHOLTZ

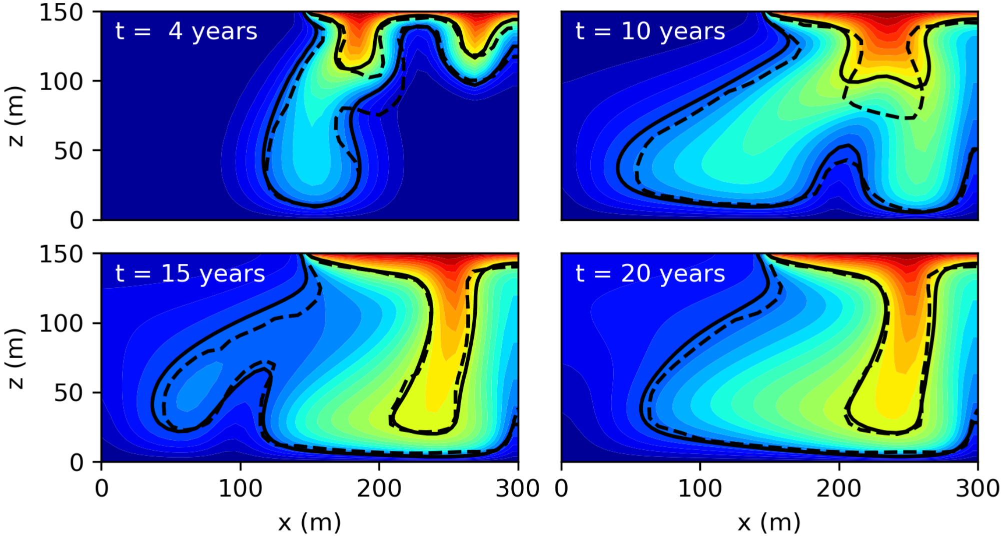
Density-driven flow Henry and Elder problems used for code validation

Henry problem describes advance of a saltwater front in a confined aquifer initially saturated with fresh water



Comparison against 0.25, 0.5 and 0.75 isochlors computed with FEFLOW and ROCKFLOW (dashed) [1]

Elder problem describes free convection with fluid flow purely driven by density differences



Comparison of simulation results (simple upwind advection scheme) against 0.2 and 0.6 isochlors computed with SHEMAT's [2] Smolarkiewicz anti-diffusion advection scheme (dashed) [3]

[1] Kolditz et al. (1998) doi:10.1016/S0309-1708(96)00034-6
[2] Clauser (2003) doi:10.1007/978-3-642-55684-5
[3] Smolarkiewicz (1983) doi:10.1175/1520-0493(1983)111<0479:ASPDAS>2.0.CO;2

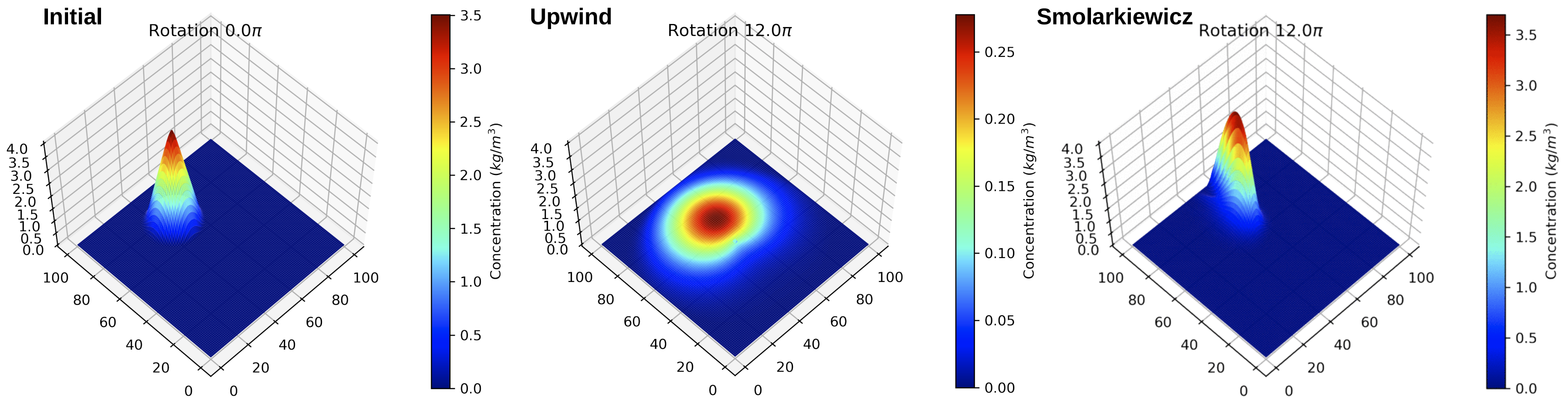
GFZ Helmholtz Centre Potsdam

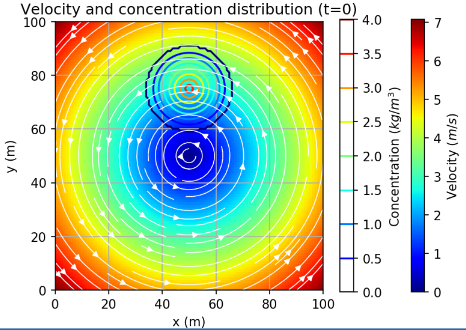
Thomas Kempka[1,2]
[1]GFZ German Research Centre for Geosciences, Fluid Systems Modelling, Potsdam, Germany
[2]University of Potsdam, Institute of Geosciences, Germany
kempka@gfz-potsdam.de

HELMHOLTZ

EGU2020-18145

Rotating cone benchmark is an advection scheme stress test for heat and species transport at extremely high Péclet numbers





Smolarkiewicz advection scheme [1] consists of two steps:
(1) simple upwind advection scheme and
(2) correction of error introduced by numerical diffusion resulting from first-order upwind scheme in step (1)

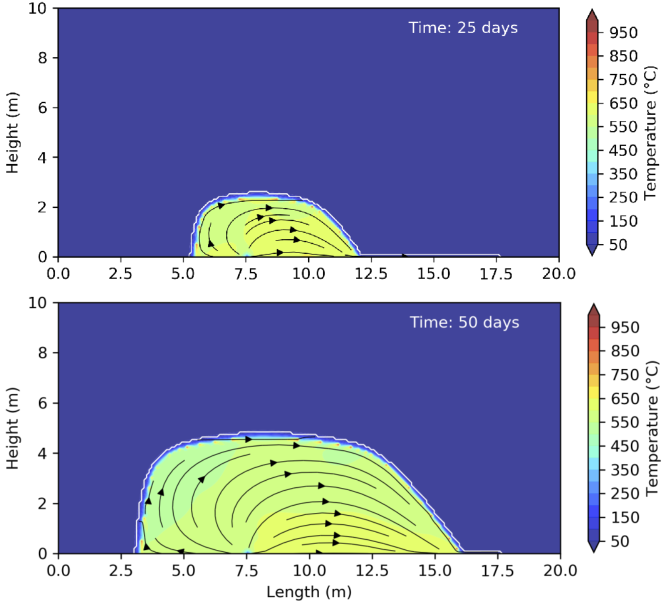
[1] Smolarkiewicz (1983) doi:10.1175/1520-0493(1983)111<0479:ASPDAS>2.0.CO;2

Thomas Kempka[1,2]
[1]GFZ German Research Centre for Geosciences, Fluid Systems Modelling, Potsdam, Germany
[2]University of Potsdam, Institute of Geosciences, Germany
kempka@gfz-potsdam.de

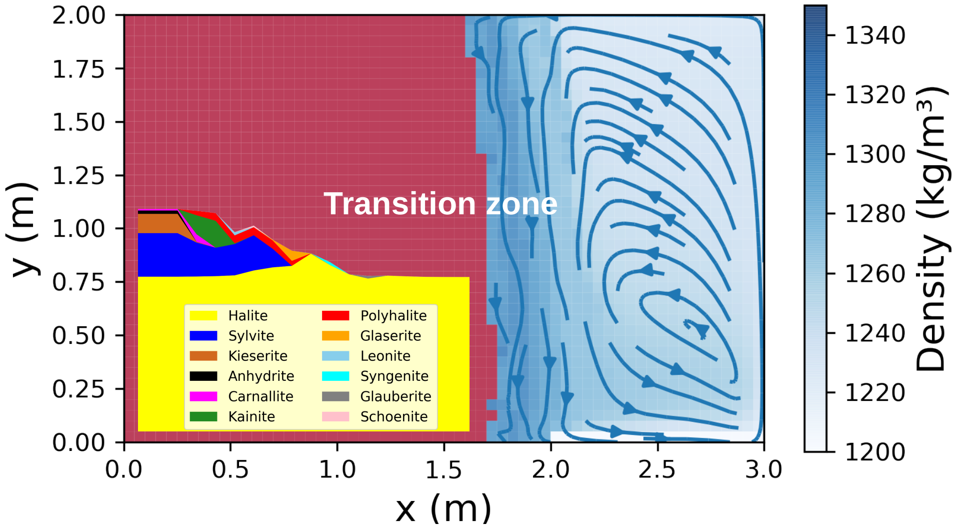
EGU2020-18145

TRANSport Simulation Environment enables flexible and efficient realisation of simulations with complex (geo-)chemical interactions

Assessing synthesis gas composition and cavity growth in underground coal gasification or subsurface coal fires



Reproducing spatial and temporal composition of transition zones within potash seams (Steding et al., EGU2020-1578)



Thomas Kempka[1,2]
[1]GFZ German Research Centre for Geosciences, Fluid Systems Modelling, Potsdam, Germany
[2]University of Potsdam, Institute of Geosciences, Germany
kempka@gfz-potsdam.de