Subflow - An Open-Source, Object-Oriented Application for Modeling Geologic Storage of CO_2*

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Abstract

The capture of carbon dioxide for its subsequent storage in brine-saturated reservoirs or depleted oil fields has become a significant part of US energy policy. In this work, we focus on the design and development of a novel CCUS application to model carbon dioxide injection in brine-saturated reservoirs. SubFlow is written in C++ and uses a relational database to store user session and simulation parameters such as mineral, solute, kinetic reaction, lithology, formation, and injection water data. Subflow is capable of 3D real-time visualization, distributed-parallel execution on massively parallel processor (MPP) systems using OpenMP and MPI, and features an intuitive user interface developed using Qt. SubFlow uses a mimetic discretization method (MDM) for solving conservation of solute mass, energy, and fluid momentum, and the finite-element method for solving the pressure, rock stress, and fracture fields. SubFlow is implemented with the Mimetic Methods Toolkit (MTK), a C++ API which allows for an intuitive implementation of the Castillo-Grone based Mimetic Discretization Methods. The FVM is second order accurate while the MDM is capable of fourth order accuracy. OpenGL is used to render pressure, temperature, stress, velocity, and solute concentration fields on a 3D mesh that represents a reservoir. Results from selected simulations are compared with those produced by TOUGHREACT and STOMP.

Selected References

Aral, M.M., and B. Liao, 1996, Analytical Solutions for Two–Dimensional Transport Equation with Time-Dependent Dispersion Coefficients: Journal of Hydrologic Engineering, v. 1/1, p. 20-32.

Bear, J., 1972, Dynamics of Fluids in Porous Media: Environmental Science Series, American Elsevier Publishing Company, 764 p.

Castillo, J.E., and G.F. Miranda, 2013, Mimetic Discretization Methods: CRC Press, ISBN 9781466513433, 260 p.

Chou L., R.M. Garrels, and R. Wollast, 1989, Comparative Study of the Kinetics and Mechanisms of Dissolution of Carbonate Minerals: Chemical Geology, v. 78, p. 269-282.

LeVeque, R.J., 2007, Finite Difference Methods for Ordinary and Partial Differential Equations: Steady-State and Time-Dependent Problems: SIAM Publications, ISBN: 978-0-89871-629-0, 328 p.

Plummer, L.N., T.M.L. Wigley, and D.L. Parkhurst, 1978, The Kinetics of Calcite Dissolution in CO_2-Water Systems at 5 to 50 °C and 0.0 to 1.0 ATM CO_2: American Journal of Science, v. 278, p. 179-216.

United States Geological Survey, The Advection-Reaction-Dispersion Equation: http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/html/final-22.html. Website accessed March 2017.

SUBFLOW

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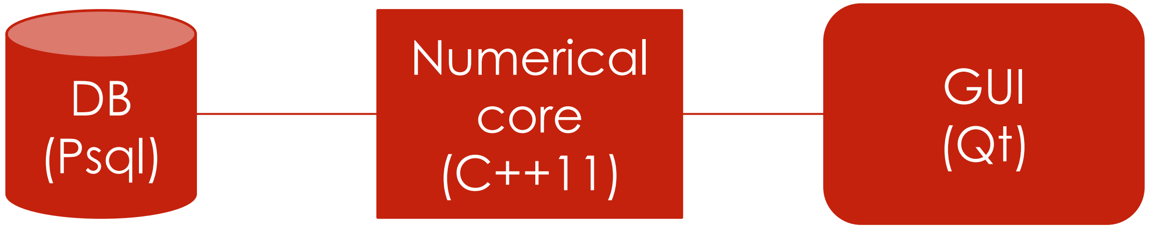
WHAT IS SUBFLOW?

SubFlow is an open source application to perform high-end subsurface flows simulations. It's main application is the modeling of Carbon dioxide sequestration in natural reservoirs. Particularly, depleted oil fields and brine water aquifers.

SubFlow is written in C++ and it is organized in the following way,



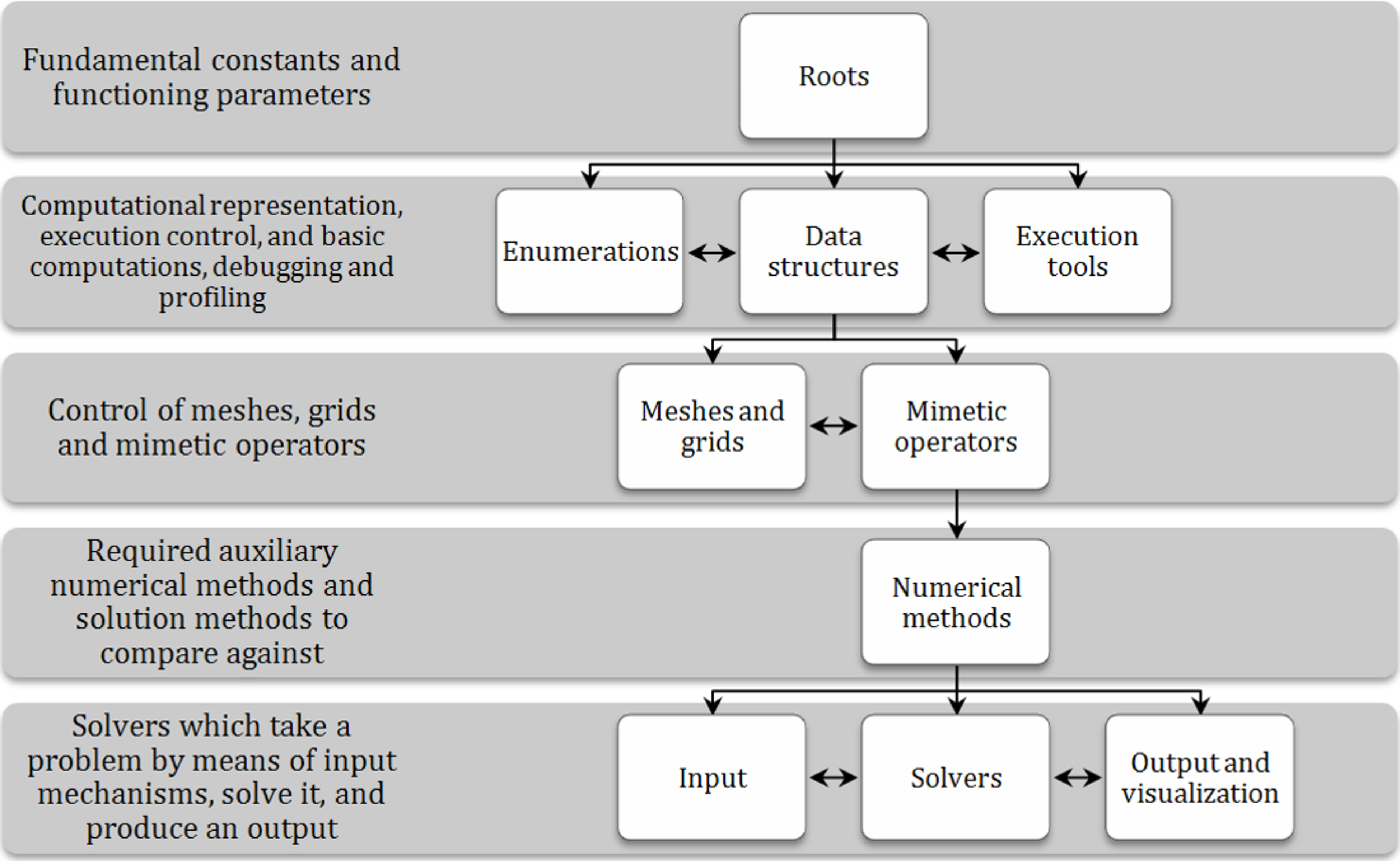
SubFlow uses the **MTK** to solve the governing partial differential equations.

WHAT IS MTK?

MTK stands for **Mimetic methods Toolkit**. It is a software library that allows users to easily solve differential equations using mimetic operators.

- It provides the four most common differential operators: $\nabla, \nabla \cdot, \nabla$x and ∇^2 with up to 8th order of accuracy
- Full support for sparse matrices operations
- It is available for **C++ and MatLab** and it depends on BLAS, LAPACK and GLPK

MTK'S TAXONOMY

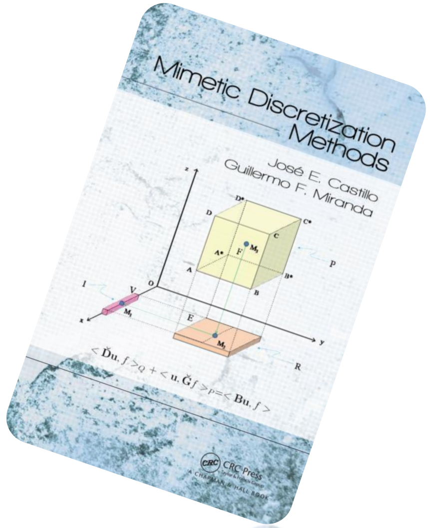


MIMETIC OPERATORS

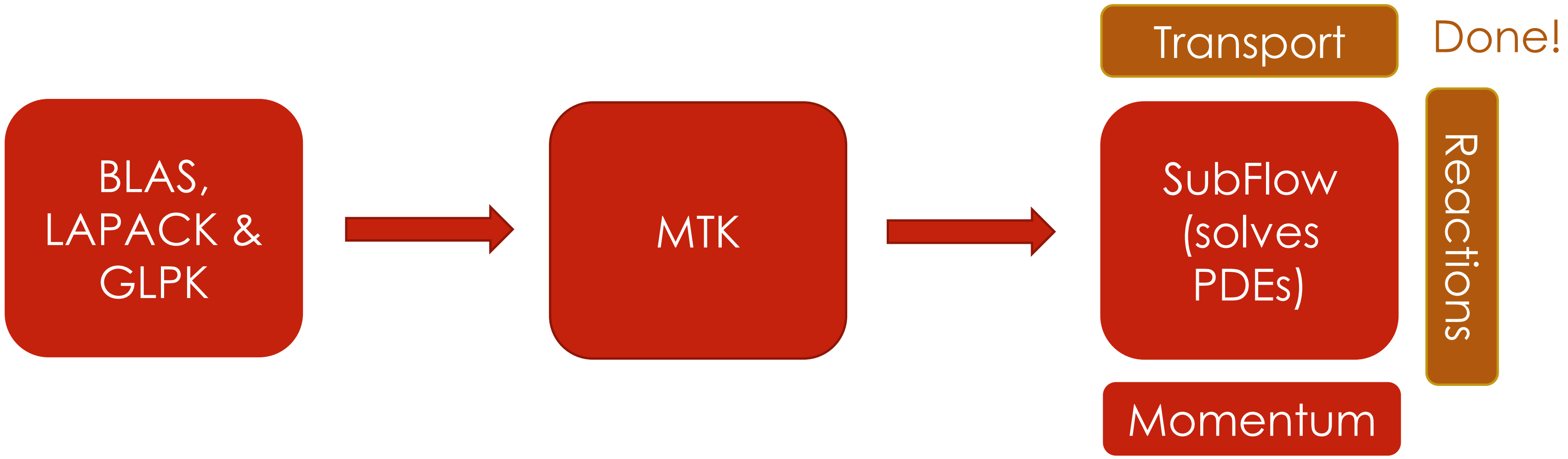
Properties

- $Dv_{const} = 0$ ✓
- $Gf_{const} = 0$ ✓
- $CGf = 0$ ✓
- $DCv = 0$ ✓
- $DGf = Lf$ ✓

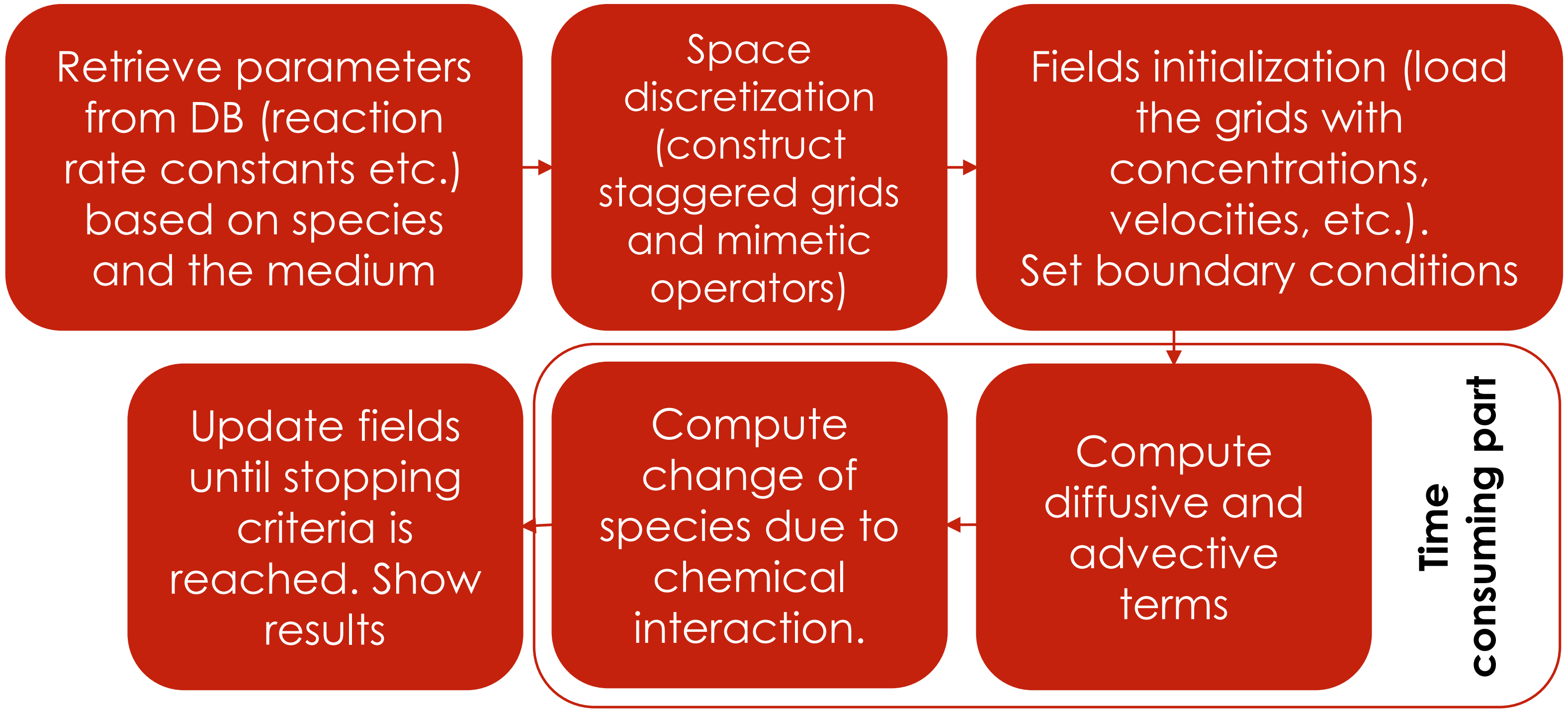
D - discrete divergence operator
G – discrete gradient operator
C – discrete curl operator
L – discrete laplacian operator



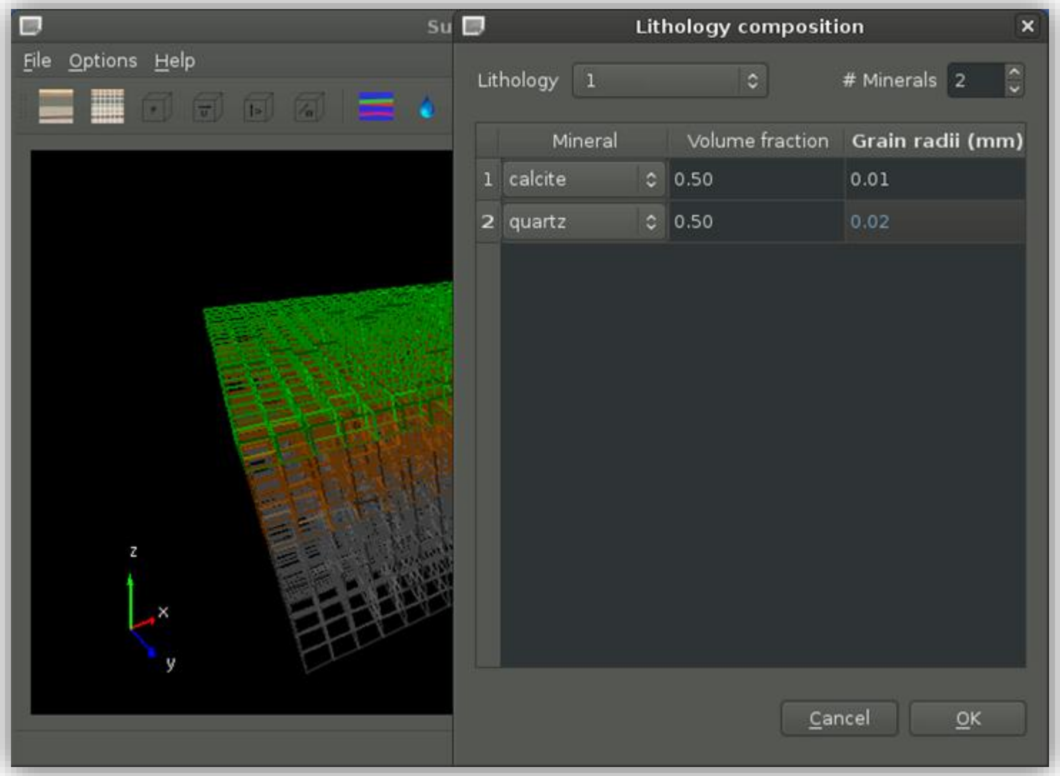
RELATIONSHIP?

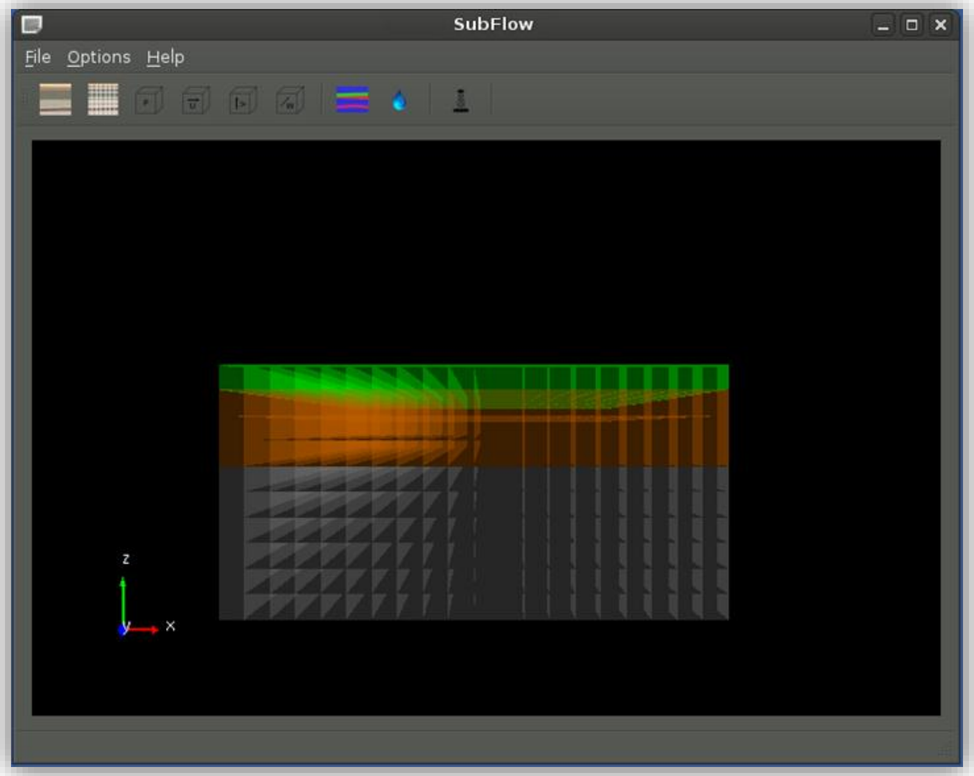


SUBFLOW'S PIPELINE

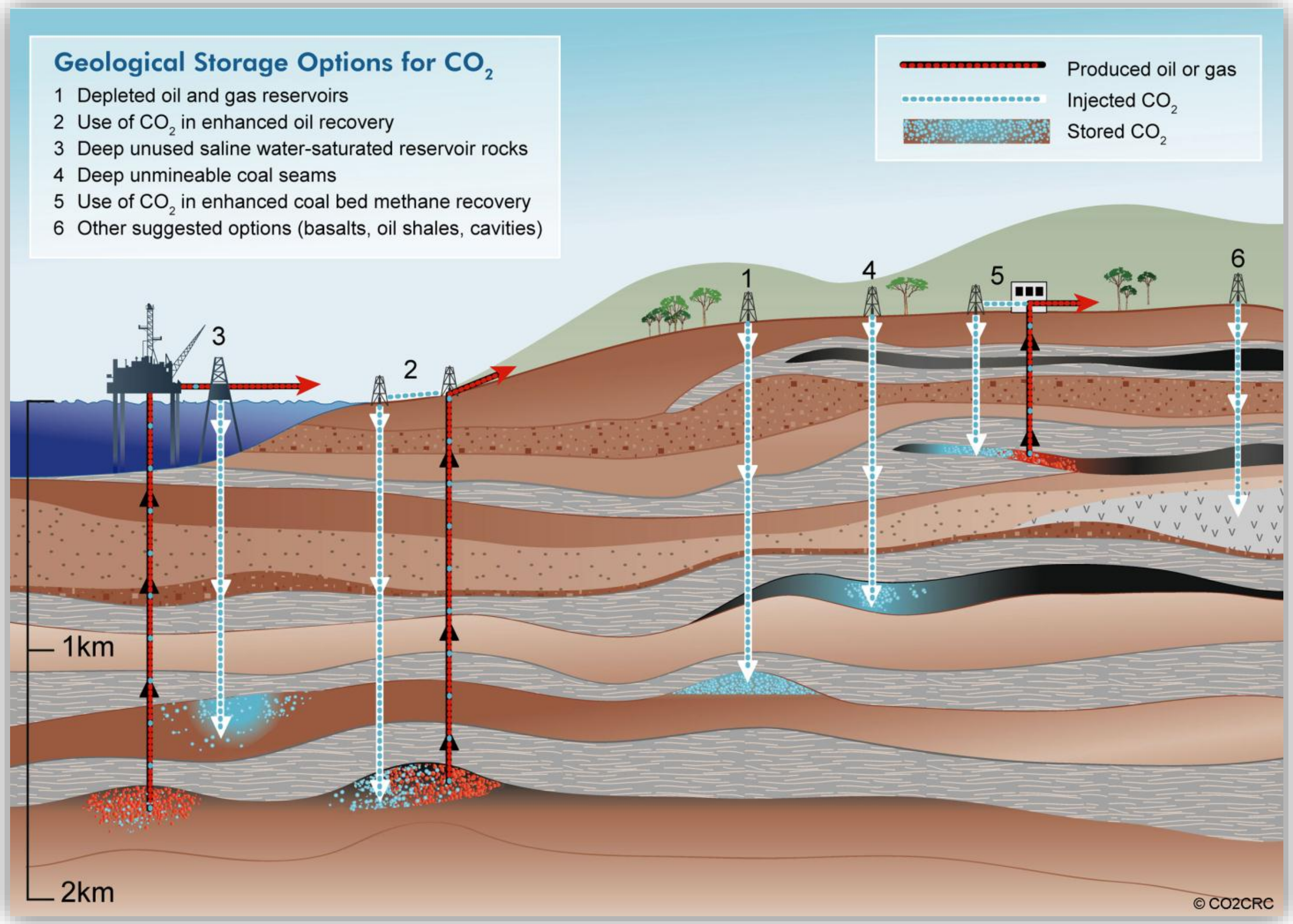


SUBFLOW'S GUI





GOAL → CO_2 SEQUESTRATION



TRANSPORT EQUATION

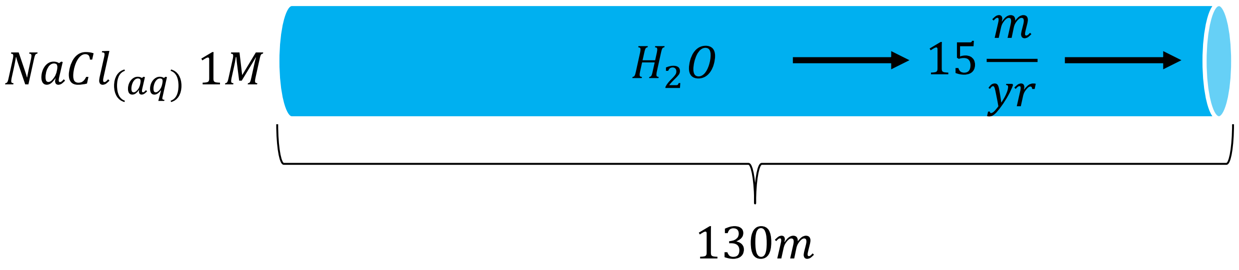
Concentration rate of change | Diffusive term | Advective term | Source term

$$\phi \frac{\partial c_\alpha}{\partial t} = \phi D_\alpha \nabla^2 c_\alpha - \phi \vec{\nabla} \cdot (c_\alpha \vec{u}) - S$$

Mimetic Laplacian operator

Mimetic Divergence operator

1-D CASE (HALITE)



Data

$$u = 15\frac{m}{yr}$$

$$\alpha_L = 5m$$

$$D_L = D_e + \alpha u$$

$$C(x,0) = 0M$$

$$C(0,t) = 1M$$

$$Na^+ \rightarrow R = 2.5$$

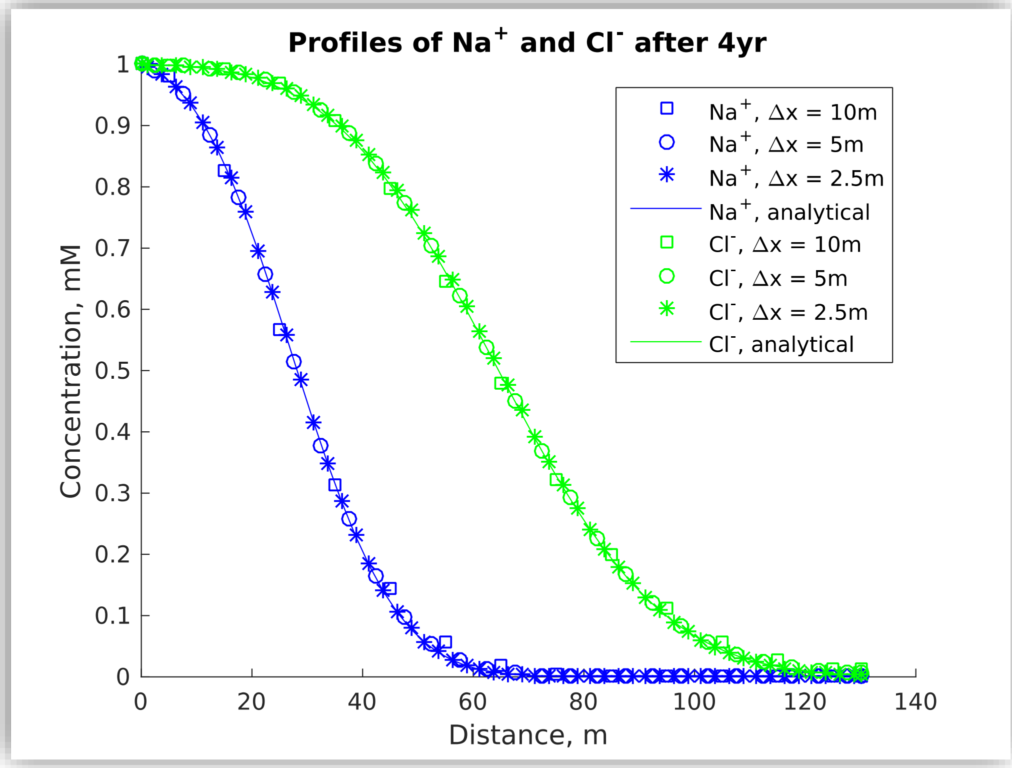
$$Cl^- \rightarrow R = 1$$

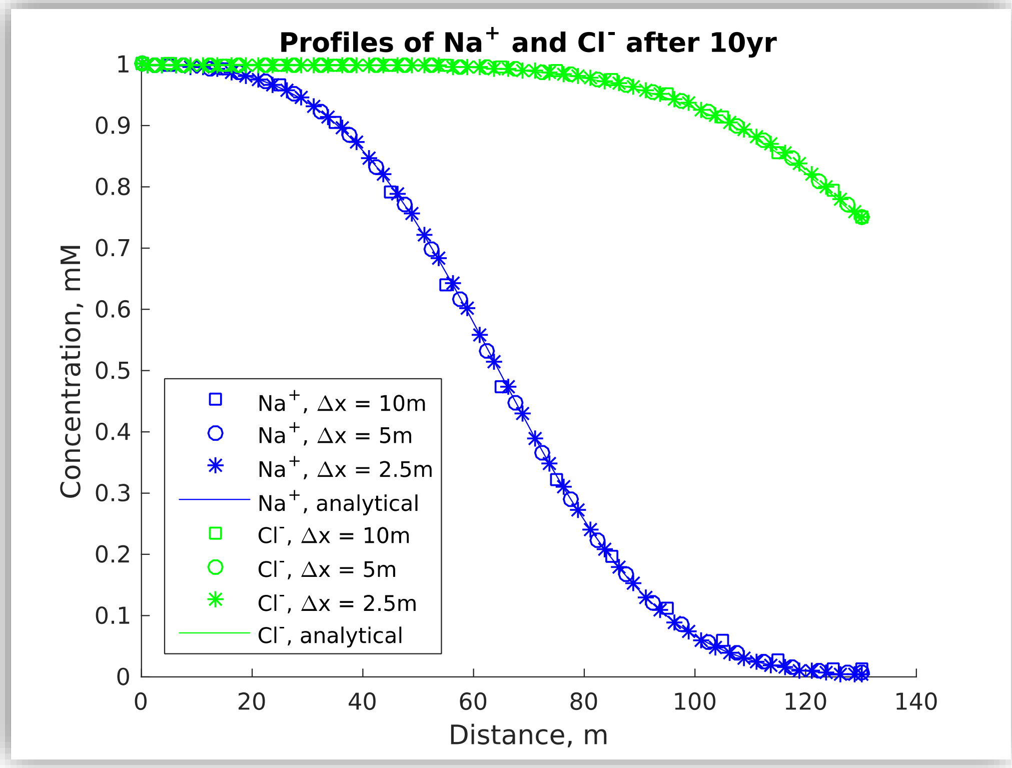
Analytical solution: $C(x,t) = \frac{1}{2}\left[\operatorname{erfc}\left(\frac{x-\frac{ut}{R}}{\sqrt{\frac{4\alpha_L ut}{R}}}\right) + e^{\left(\frac{x}{\alpha_L}\right)}\operatorname{erfc}\left(\frac{x+\frac{ut}{R}}{\sqrt{\frac{4\alpha_L ut}{R}}}\right)\right]$

erfc is the complementary error function.

From: http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/html/final-22.html

1-D CASE - RESULTS

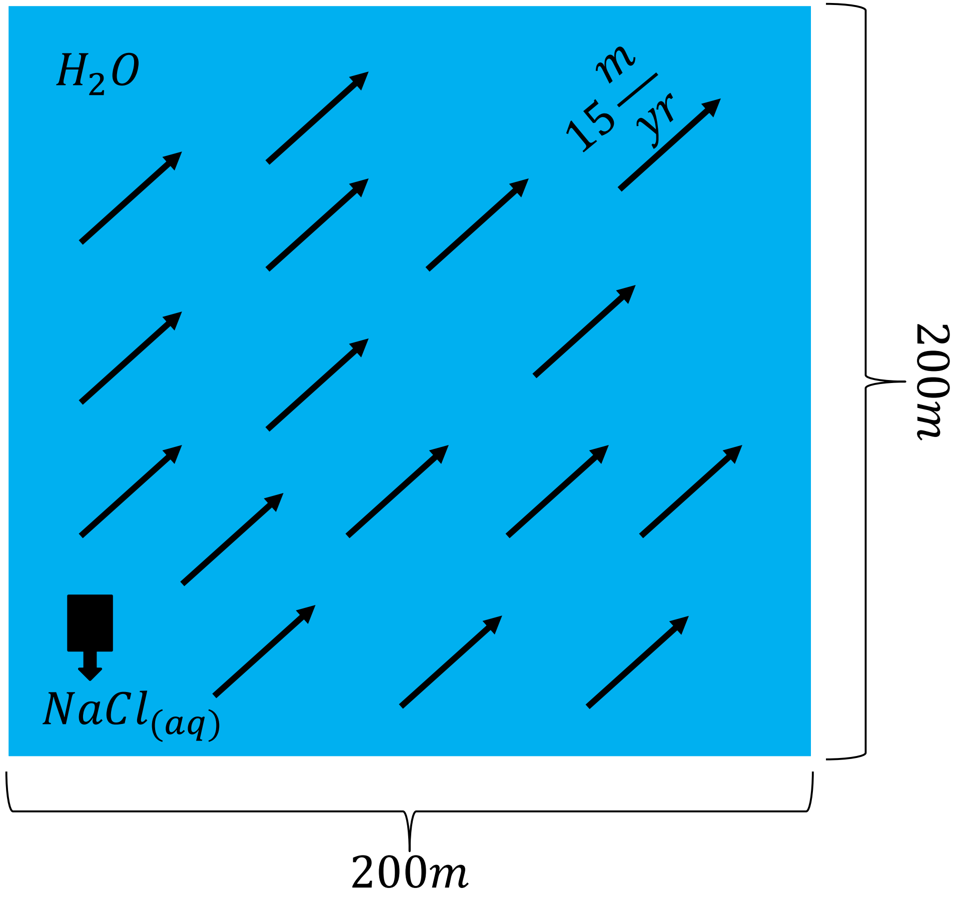




2-D CASE (HALITE)

$$C(x,y,t) = \frac{aM}{4\pi\phi\sqrt{D_L D_T}\frac{t}{R}} e^{\left[-\frac{\left(x-\xi-\frac{u}{R}t\right)^2}{\frac{4D_L t}{R}} - \frac{\left(y-\eta-\frac{v}{R}t\right)^2}{\frac{4D_T t}{R}}\right]}$$

Analytical solution



Data

$u = 15\frac{m}{yr}$

$v = u$

$D_T = D_L = 75\frac{m^2}{s}$

$C(x,y,0) = 0M$

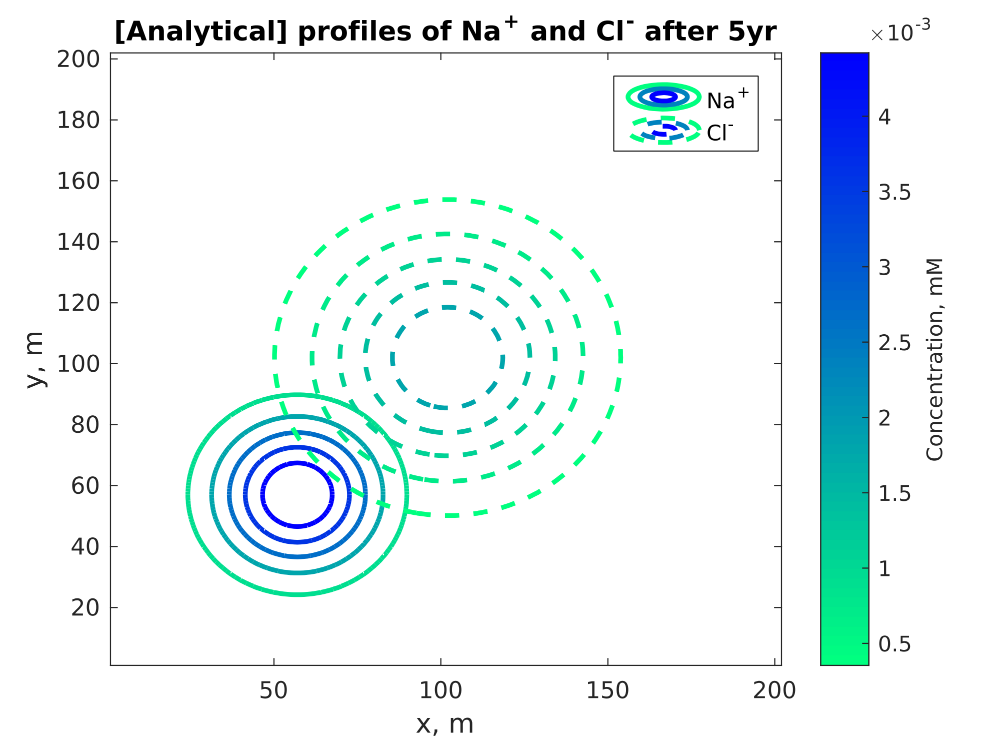
$C(25.5,25.5,0) = 10M$

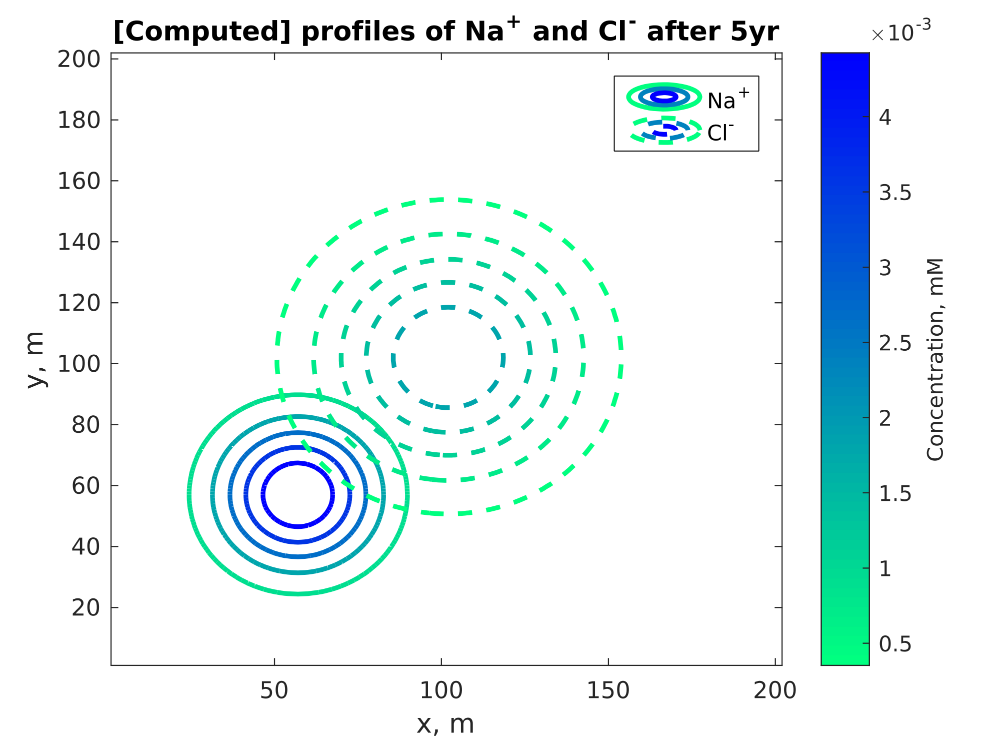
$Na^+ \rightarrow R = 2.5$

$Cl^- \rightarrow R = 1$

From: "Dynamics of fluids in porous media" by Jacob Bear

2-D CASE - RESULTS





$\Delta x = \Delta y = 1m$

2-D CASE (TRACER)

Injection of a tracer with radioactive decay.

Data

$$u = 5\frac{m}{s}$$

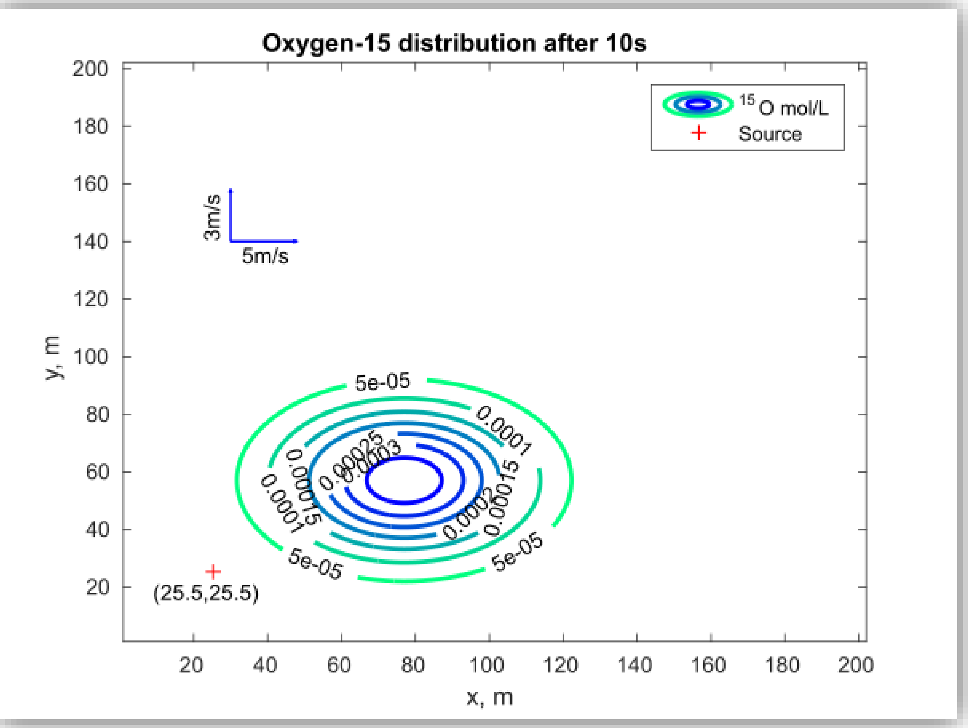
$$v = 3\frac{m}{s}$$

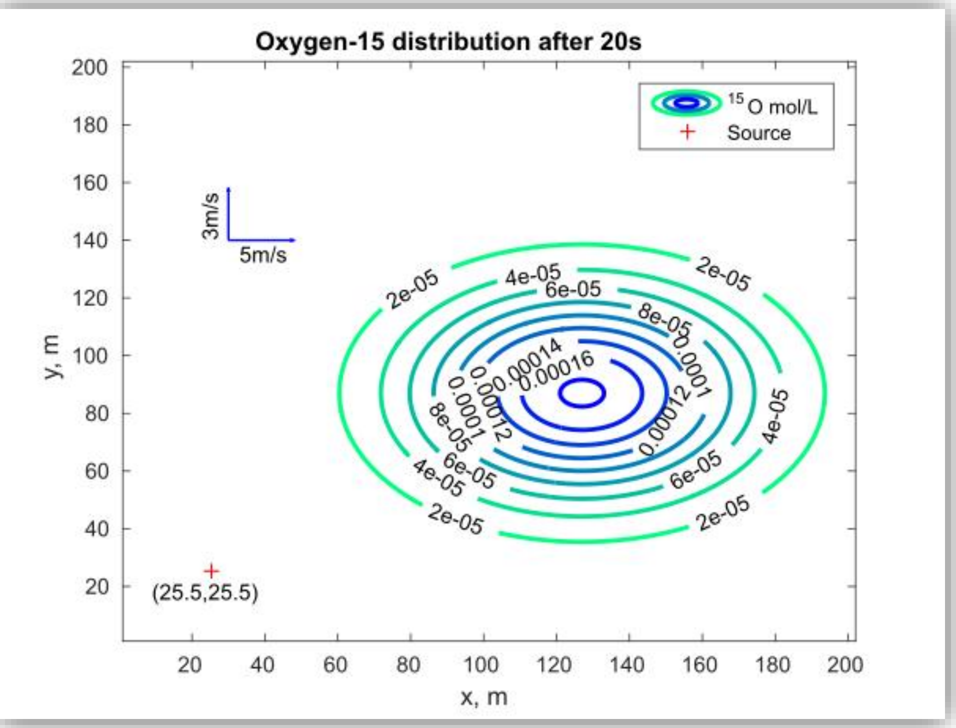
$$\alpha = 5m$$

$$\lambda = 0.0057s^{-1}$$

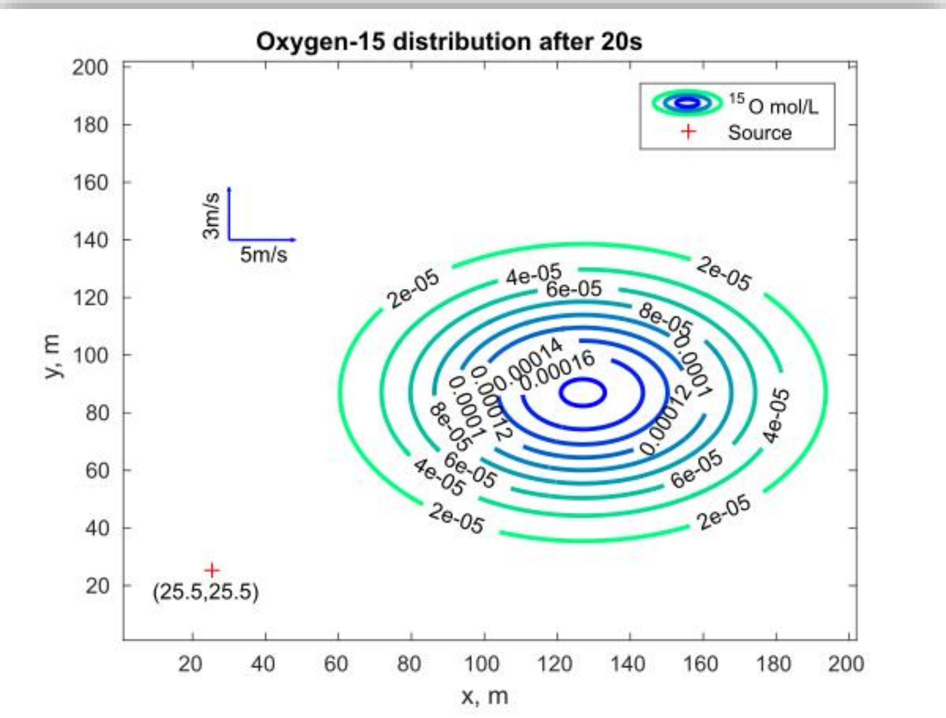
$$C(x, y, 0) = 0M$$

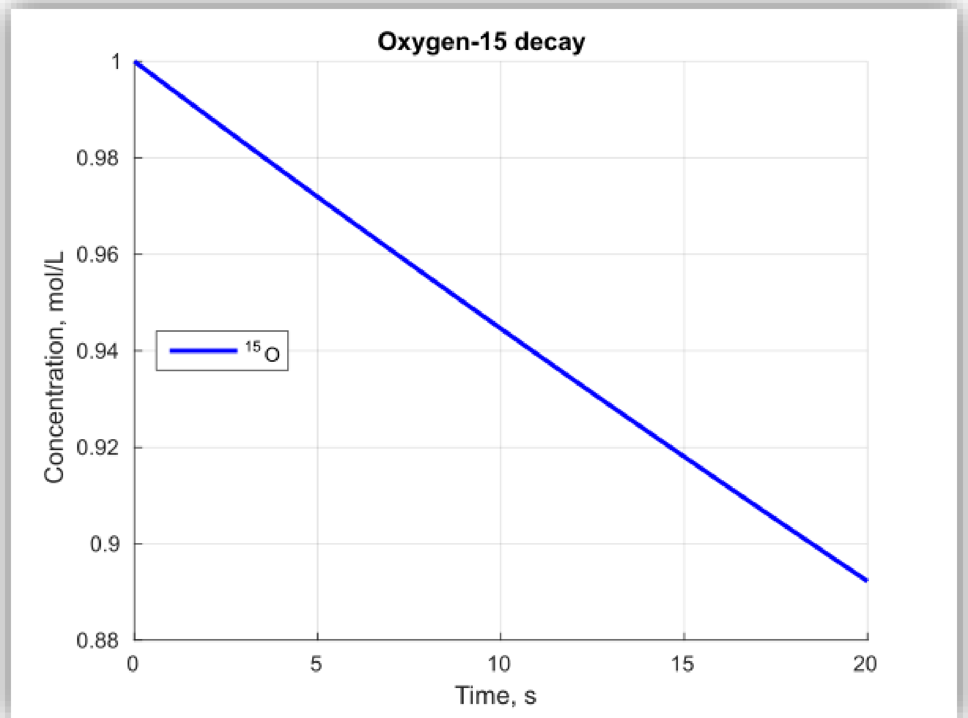
$$C(25.5,25.5,0) = 1M$$





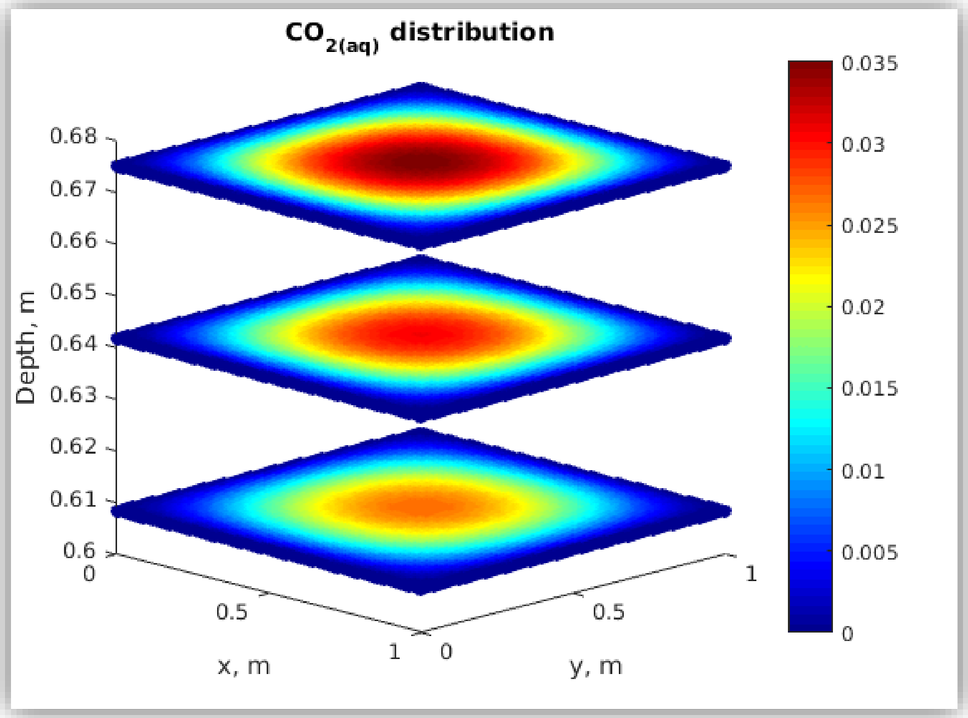
2-D CASE (TRACER)



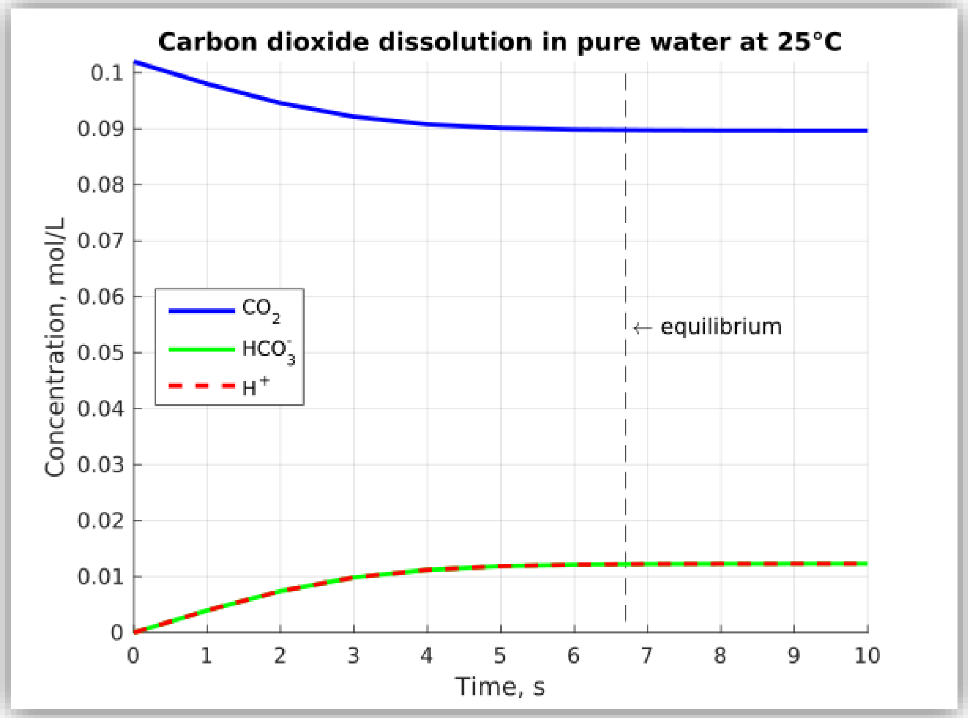


3-D CASE (CARBON DIOXIDE)

$[CO_2(aq)]_0 = 0.102M$



Source term



Obtained using 3-D mimetic operators!

FUTURE WORK

- 3-D capability (in progress)
- Variable velocity fields (momentum)
- Multiphase transport
- Hybrid parallel implementation
- Coupling with fractures' module (Jonathan Matthews' work)

REFERENCES

- Analytical Solutions for Two-Dimensional Transport Equation with Time-Dependent Dispersion Coefficients. Mustafa Aral et al. Journal of Hydrologic Engineering, 1996
- Dynamics of Fluids in Porous Media. Jacob Bear. Elsevier, Environmental Science Series, 1972
- The Advection-Reaction-Dispersion Equation. United States Geological Survey
- The Kinetics of Calcite Dissolution in CO_2-Water Systems at 5° to 60 °C and 1 ATM CO_2. N. Plummer et al. American Journal of Science, 1978
- Comparative Study of the Kinetics and Mechanisms of Dissolution of Carbonate Minerals. Lei Chou et al. Elsevier, Journal of Chemical Geology, 1989
- Mimetic Discretization Methods. Jose E. Castillo & Guillermo F. Miranda. CRC Press, 2013
- Finite Difference Methods for Ordinary and Partial Differential Equations. Randall J. LeVeque. SIAM, 2007

THANK YOU!