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Analytical Benchmark to Test Numerical Modelling of Spatial Distribution of Root Exudations in Soils with Dumux

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Different types of root exudates and their effect on soil/rhizosphere properties have received a lot of attention. Since their influence on rhizosphere properties and processes depends on their concentration in the soil, the assessment of the spatial-temporal exudate concentration distribution around roots is of key importance for understanding the functioning of the rhizosphere.

Accurate modelling of spatial distribution of root exudates in the soil offers insights into achieving better interpretation and prediction of spatial distribution of root exudates. Meanwhile, compared with experimental research, mathematical simulation is flexible in time and economical.

Accurate mathematical simulation of root exudates transport in the soil requires a correct representation of underlying mechanisms in a mathematical model. The accuracy of simulation is equally determined by the correctness of equations of mathematical equations. Due to the universally existed nonlinearity and complex boundary conditions, the numerical approximations are considered as major method to solve complicated mathematical equations.

In this paper, we evaluate the numerical models implemented in DuMux, which is an open source simulator for simulating flow and transport in porous media. We consider a simplified root architecture where each root is represented by a straight line. Assuming that root tips move at a constant velocity and that exudation transport is linear, concentration distributions can be obtained from the convolution of the analytical solution of the transport equation for a moving point or line source injection. By coupling the analytical solution with a root growth model that delivers the spatial-temporal pattern of root distribution in 3D space, we simulated exudate concentration distributions for citrate and mucilage with CRootBox. Based on analytical solutions, our purpose is to define benchmark scenarios to verify the accuracy of numerical solution.

From the simulation results, we inferred the following information about numerical solution: (a) coupled transport equations implemented in DuMux is capable of simulating the spatial distribution of root exudates; (b) Numerical solutions are much adaptive for nonlinearity problems compared with analytical solutions for the transport of root exudates in the soil. In future work, we will use the simulation tool to infer critical parameters that determine the spatial-temporal extent of the rhizosphere from experimental data.