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An objective-oriented tool to model biogeochemical degradation of emerging organic contaminants in porous media

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The increasing of emerging organic contaminants in surface and subsurface aquifer system threatens the health of human beings and ecosystems. Reactive Transport modeling can be used to predict degradation processes of organic matter, as controlled by physical and biochemical mechanisms. However, microbial-mediated chemical reaction is kinetically complex and leads to complicated non-linear problem. The problem is further hindered by the limited understanding of the degradation process which is catalyzed by numerous types of microorganisms that play complementary functions and adapt to evolving conditions such as the redox sequence. Accounting for all these factors makes conventional procedure-oriented codes no longer suitable. Therefore, an objective-oriented modern Fortran module is designed to explore microbial mediated reactive transport process.
The module consists of two main classes. The chemical system class imitates reactions within same phase (homogeneous reactions) and between different phases (heterogeneous reactions) and depicts the thermodynamic activity of species involved in phase. In such a way, the increased complexity of biogeochemical degradation system can be simplified by the establishment of individual microorganism community phases. The local chemistry class captures physical biogeochemical states variables and encapsulates procedures such as speciate and mixing. It provides a way to diversify the polymorphism chemical system exists on each mesh node. These two classes can be used as an independent module to couple extensive chemical processes with multi-physical phenomena (flow, solute transport, heat transport, etc.) governed by partial differential equations. It has been illustrated that the innovative module can be easily implemented into conservative transport code. By applying water mixing approach (WMA) instead of direct substitution approach (DSA) and sequential iteration approach (SIA) to solve kinetic-equilibrium reactive transport improve computational efficiency while ensuring simulation accuracy.