

## **Coupling KBASE with PFLOTRAN**

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<https://www.subsurfaceinsights.com/microbiological-with-pflotran>

### **Project Goals: Short statement of goals. (Limit to 1000 characters)**

The goal of this project is to develop a high throughput, semi-automated data and analytical pipeline which will allow the use of the PFLOTRAN reactive transport modeling system in conjunction with KBase to model microbiological processes within an ecosystem.

### **Abstract**

Watersheds are complex hydrobiogeochemical systems which provide multiple ecosystem services which are essential for US energy, food and water security. The manner in which watersheds provide these services is through a complex combination of the behavior of different watershed components (e.g. vegetation, soil, surface water) across a range of spatially nested subunits.

A predictive, actionable and science-based understanding of watershed behavior is critical for managing watershed resources and services. Achieving this understanding is extremely challenging due to various complex interactions within a watershed between plants, microorganisms, organic matter, soil, and water as well as the wide range of spatial and temporal scales across which these interactions take place. This challenge is exacerbated as these multi-scale interactions vary over time as a function of landscape position, elevation, human activity, environmental and biogeochemical gradients, and multiple feedback loops. While historically efforts to develop this understanding have focused on physical and chemical processes, there is a growing recognition that we need to develop a better understanding of hydrobiogeochemical processes. This will require the integration of physical, chemical and microbiological watershed data and coupling and integration of analytical tools and models across multiple domains, and should be done through a pipeline which has both data and analysis components. The data component should bring together the datasets required for such an understanding which are then used by the analysis component for the outcome of actionable information on hydrobiogeochemical processes.

Such a pipeline should be robust, semi-automated, high throughput and be useable by scientists from multiple domains.

Our approach in implementing this pipeline has been to develop cloud based software which provides a coupling between KBase (<https://kbase.us/>) and the open source reactive flow and transport modeling code PFLOTRAN (<https://www.pflotran.org/>). Our approach leverages and builds on the existing capabilities in these software packages, and specifically uses the Flux Balance Analysis capabilities in KBase to generate the input reactions which can be used by PFLOTRAN to simulate the geochemical processes driven by the microbiological species present in the subsurface.

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