

Reactive Transport Modeling Tutorial Session #2

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Subsurface
Insights

Session objective

1. Present challenge of and possible approach to scaling of reactive transport modeling of microbial processes
2. Introduce hands on online modeling tutorial with interactive reactive transport modeling
3. Discuss and present pipeline for automated microbial modeling using KBASE and PFLOTRAN

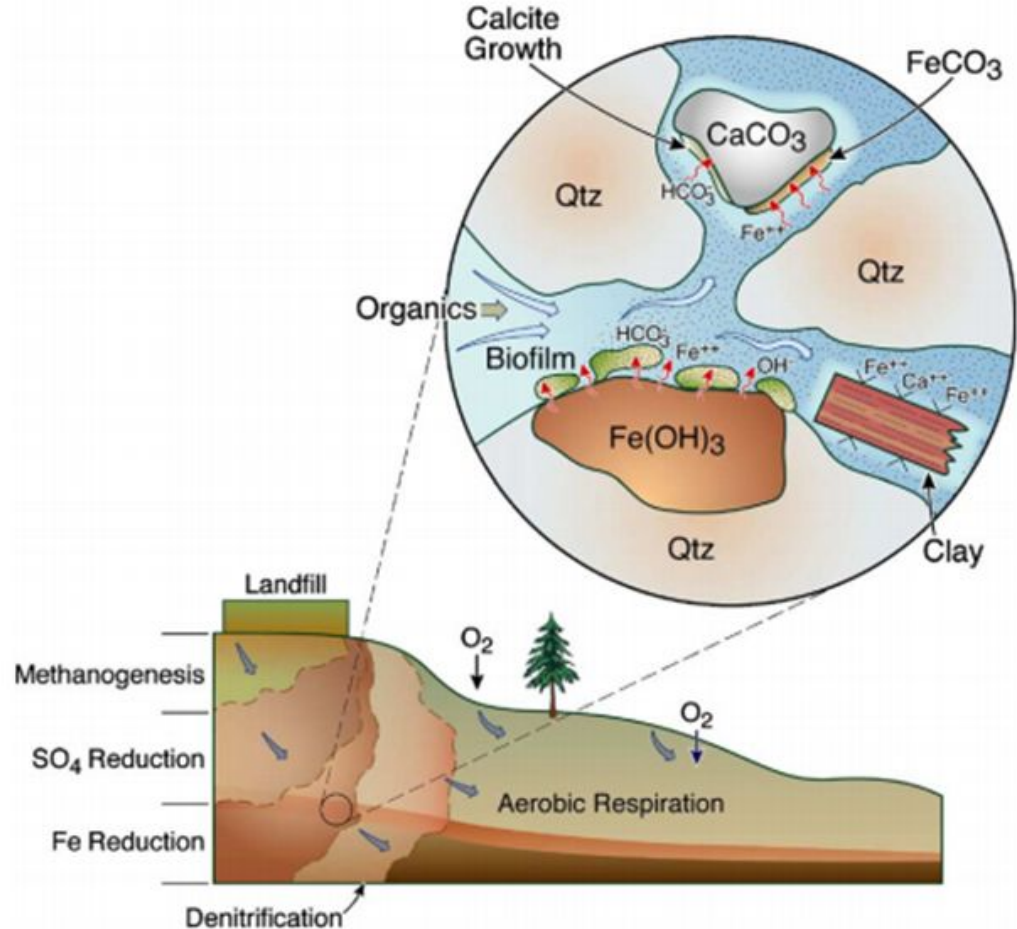
Why use reactive transport models for microbial modeling?

- Microbes exist in space and time
- Modeling of microbial processes needs to consider macroscopic spatial and temporal dynamics (fluxes of temperature, moisture and chemicals)
- Reactive Transport models are designed for this

Steefel, de Paolo and Lichtner 2005

Oxidation/Reduction Zones that may develop in aquifer downstream from organic rich landfill:

- Methanogenesis
- Sulfate reduction
- Dissimilatory iron reduction
- Denitrification
- Aerobic respiration



Scaling challenge:

After the workshop, all attendees would like to model microbial dynamics

- At multiple spatial scales
- At multiple temporal scales
- In multiple dimensions
- At multiple locations



There may be millions of models we collectively would like to build and run!

Big question: How do we scale our modeling capabilities?

Mismatch between data generation and model generation capabilities



Data generation



Model generation

Why is scaling hard ?

1. Acquiring understanding of what is involved in modeling is complex
2. Assembling data for models (geochemical, microbiological, hydrological, environmental) is time and labor consuming
3. Building and running microbial models is complex

Why is scaling hard

1. Acquiring understanding of what is involved in modeling is complex
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What can we do about it?

1. Make it easier to acquire a basic understanding of modeling
2. Develop and provide data management automation, discovery and access mechanisms
3. Create a microbial modeling pipeline that uses KBASE and PFLOTRAN so that we can easily create and run models

Remainder of presentation

1. Introduce online, hands on tutorial which should allow attendants to understand key aspects of modeling
2. Briefly discuss aspects of data management, discovery and access mechanisms
3. Demonstrate results of a microbial modeling pipeline that uses KBASE and PFLOTRAN

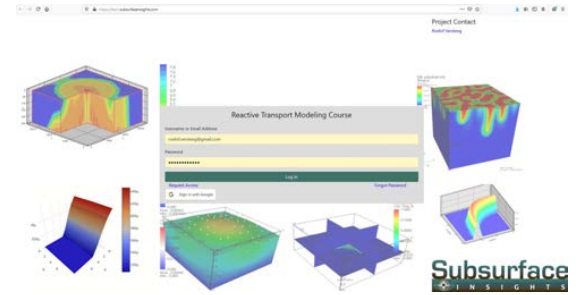
Online modeling course

Development motivated by need for educated collaborators -> collaborators do not need to become modelers, but need to understand modeling basics

Key part: interactive, hands on modeling to provide intuitive insights

Low activation energy:

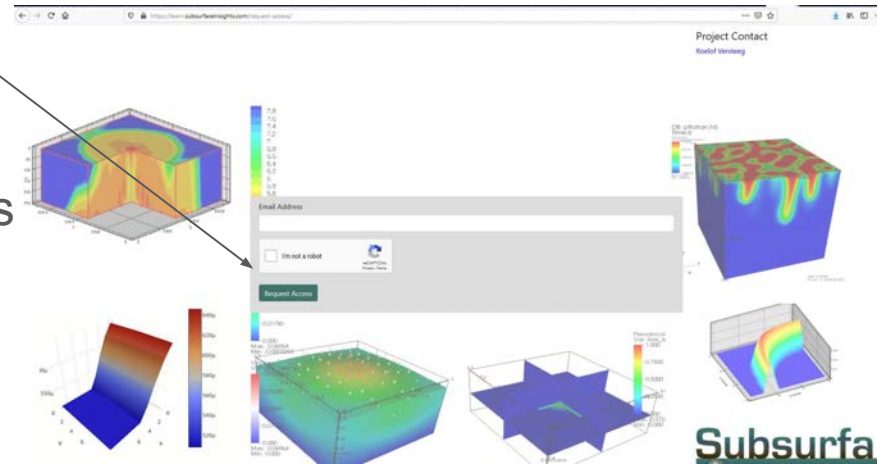
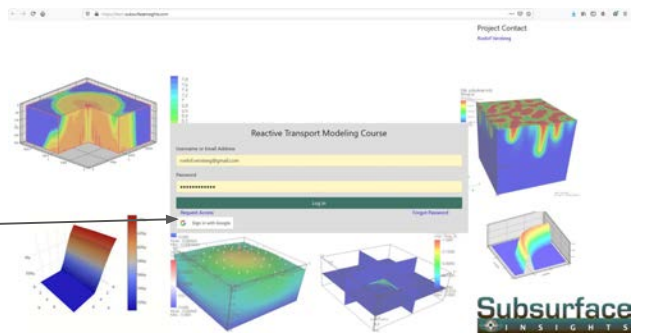
- no need to install PFLOTRAN
- Intuitive GUI



Development of this course was funded under DOE SBIR award DE-SC0015145 by the United States Department of Energy, Office of Science Advanced Scientific Computing Research to Subsurface Insights (PI Dr. Haiyan Zhou)

To get access

1. Go to <https://learn.subsurfaceinsights.com>
2. Hit request access button
3. Brings up second window
4. Enter email, and click request access (make sure to confirm you are not a robot)
5. You will get a registration link
6. We will start sending out registration links after going through course overview (so 15-20 minutes into talk)



Course

- Meant to provide comprehensive introduction to reactive transport modeling
 - General overview of modeling and visualization concepts
 - Chemistry
 - Flow and transport
 - Numerical modeling
 - PFLOTRAN basics
 - Details on PFLOTRAN infile model building
- Throughout course: Interactive PFLOTRAN modeling

**Send course comments/suggestions/bugreports to
learn@subsurfaceinsights.com**

Subsection

The screenshot shows a web browser window with the URL learn.subsurfaceinsights.com/learn/#0.0.2.course-navigation-and-interactive-modeling. The page title is "Learn | Subsurface Insights".

Section: A vertical sidebar menu on the left side of the page lists various course sections. The "Introduction" section is highlighted with a blue background. An arrow points from the label "Section" to this menu.

Subsection: A horizontal top navigation menu contains several subsections: "About this course", "What are numerical models and what do they do?", "Course Navigation and Interactive Modeling" (which is the active subsection), "PFLOTTRAN", "Acknowledgements", "Disclaimer and Legal Notices", and "About Subsurface Insights". An arrow points from the label "Subsection" to this menu.

The main content area displays the following sections:

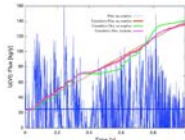
- Course Navigation and Interactive Modeling**
Depending on the pre-existing knowledge of the student, this course should take between 5 and 15 hours. The material is presented sequentially with modules building on top of one another, but students are free to move ahead or circle back. Some details on navigation are given below.
- Course navigation**
The navigation menu on the left hand side of the course page includes Chapters and Sections. In any given Section, Subsections are in the top menu. Equations and Reactions are numbered throughout the course to aid in finding and referencing these. Equation numbers are in the form "#.#.#.#" and Reactions are designated with "R.#.#.#" where the numbers are the chapter, section, subsection, and equation/ reaction within that subsection.
- Browser requirements**
The course was tested on the latest versions (June 2020) of Chrome and Firefox. It may work on other browsers.
- External links**
Hyperlinks to different external resources are provided at multiple places in the text. Two kinds of links are provided: links to other webpages (which should open in a separate window) and links to articles and reports in PDF form. Dependent on your browser configuration clicking the latter link can either open a PDF in a separate window or start download. Where we provide a link to a PDF article and report we indicate this in the text.
- Units and Dimensions**
In this course, dimensions (non-numerical physical properties) will be specified in square brackets and units (names for measurements used on those dimensions) will be specified in parentheses. For dimensions, the following abbreviations are used:
 - Mass (M)
 - Length (L)
 - Time (t)
 - Temperature (T)Note that some parameters are dimensionless (-) and unitless [-], which is specified in place of units or dimensions for those parameters.
- Glossary of Symbols**
Because of the range of topics covered in this course, which are used by a wide variety of fields that often use different symbology, we have included a Glossary of Symbols in the course Appendix. You

Section

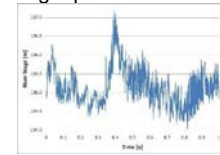
Navigation through side menu (sections) and top menu (subsections) should be intuitive

Key piece of course: PFLOTRAN

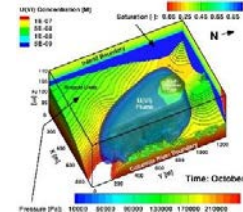
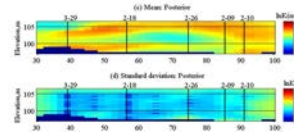
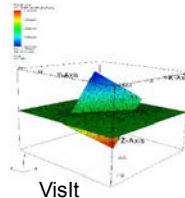
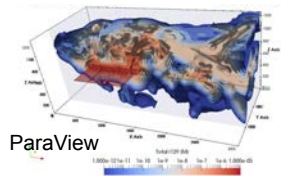
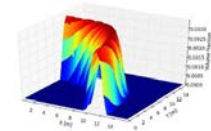
- PFLOTRAN: open source, massively parallel subsurface flow and reactive transport modeling software
- Developed by DOE scientists at different national labs since 2000
- Simulates transport and reactions in either 0, 1, 2 or 3 D
- <https://www.pflotran.org/>



gnuplot



Excel

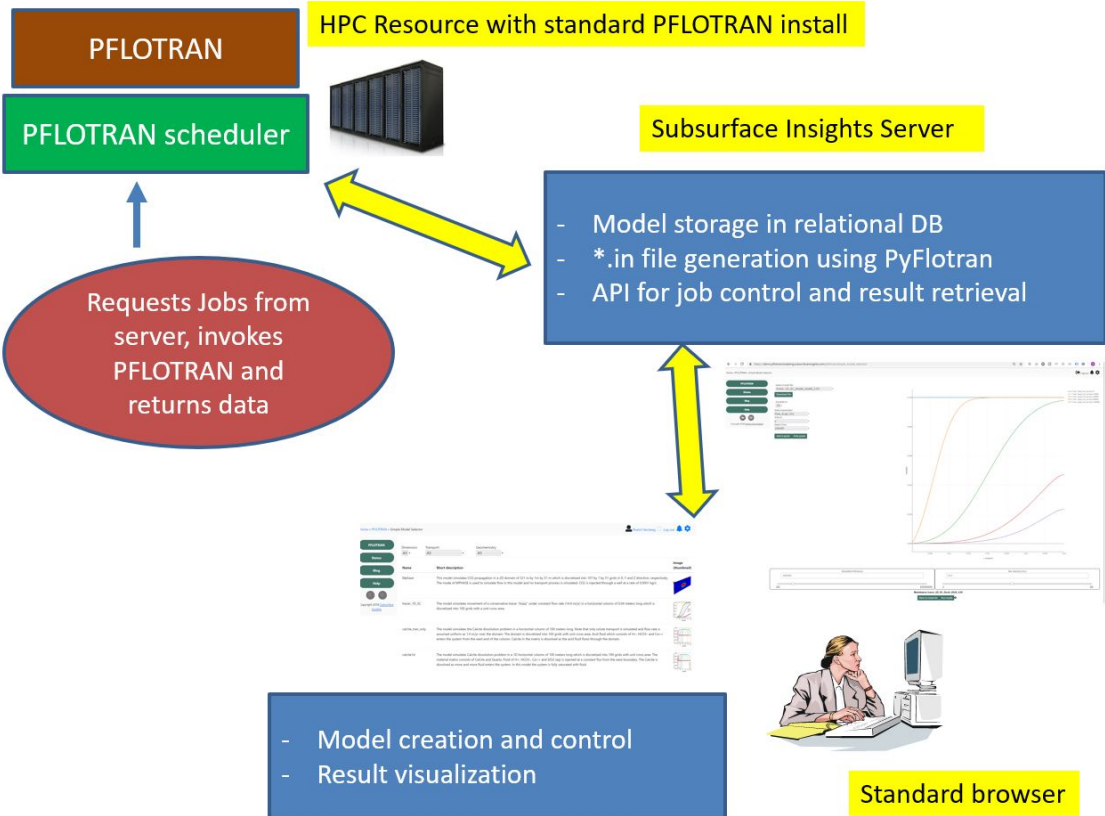


PFLOTRAN capabilities

- Transport
 - Saturated and unsaturated flow
 - Multicomponent
 - Mobile/immobile primary species
 - Advection (upwinding)
 - Hydrodynamic dispersion
- Reaction
 - Aqueous speciation
 - Ion activity models
 - General ($A + B \leftrightarrow C$)
 - N^{th} order kinetics
 - Reversible
 - Mineral precipitation-dissolution
- Microbiological
 - Michaelis–Menten kinetics
 - Biomass
 - Inhibition
- Radioactive decay with daughter products
- Sorption
 - Isotherm-based: linear, Langmuir, Freundlich
 - Ion exchange
 - Surface complexation
 - Equilibrium
 - Kinetic / multirate kinetic
- Reaction Sandbox

PFLOTRAN is well suited for modeling microbiological processes - challenge is steep learning curve

Solution - expose models through a browser (mechanism used in course)



Architecture allows

- a) Expose model parameters
- a) programmatic model building and modification

Course housekeeping

Once you get an account, for now please turn off Auto-run and sweep models

Send comments/issues to learn@subsurfaceinsights.com

Interface uses currently stable PFLOTRAN version (v2). Will upgrade to v3 in coming month.

Registered users will be on a low volume mailing list with course update information

The image shows a screenshot of a web interface. At the top, there is a rounded rectangular box containing the text 'Appendix'. Below this box is another rounded rectangular button labeled 'Options'. Underneath the 'Options' button are two checkboxes, each followed by text: the first is an unchecked checkbox followed by 'Auto-run models', and the second is an unchecked checkbox followed by 'Sweep models'.

Models and model output basics

Models have dimensionality in space and time:

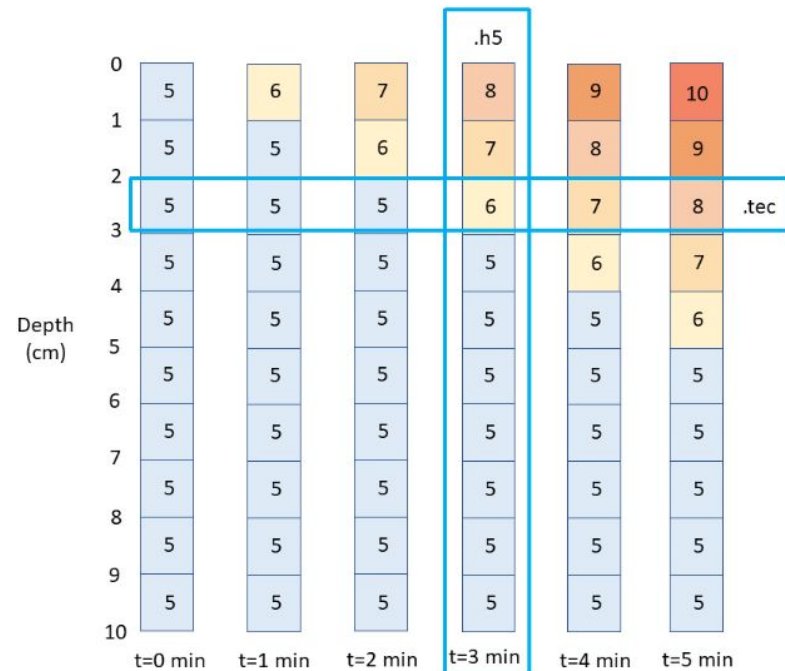
- we can model in 0,1,2,3 D
- We can model either in time T (1T) or instantaneously (0T)

Models range from 0D, 0T to 3D, 1T

Different models provide different understanding

Key point - understanding model output

- <https://learn.subsurfaceinsights.com/learn/#1.1.2.visualization-in-time-and-space>
- We can output and visualize in different ways
- Example
 - 1D, 1T model
 - Column with ten blocks of 1 cm each
 - We model the evolution (e.g. thermal diffusion)
- We can look at
 - One location for all times (tec file)
 - All locations for one time (h5 file)
- PFLOTTRAN can generate both files

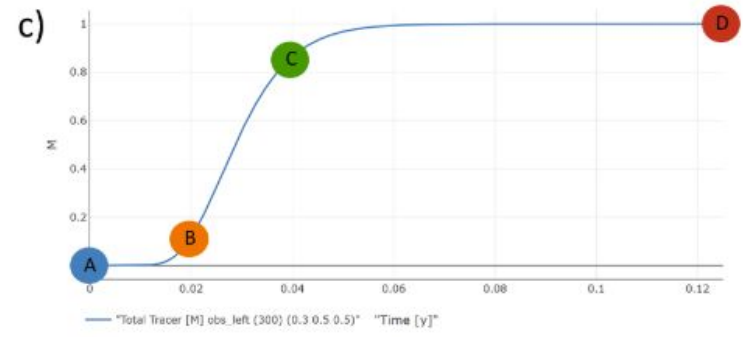
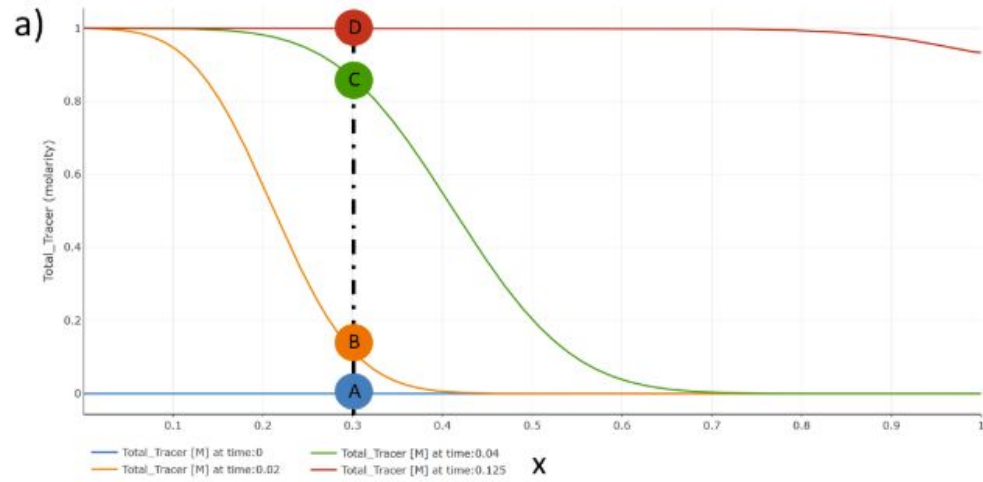


Same model

Different visualization

- Space (top)
- Time (bottom)

Both provide insights



Simplest model: 0d,0-t - Aqueous Complexation

<https://learn.subsurfaceinsights.com/learn/#2.1.0.water-chemistry>

Detailed PFLOTRAN
description

The screenshot displays the Subsurface Insights web interface. At the top, the browser address bar shows the URL <https://learn.subsurfaceinsights.com/learn/#2.1.0.water-chemistry>. The page title is "Learn | Subsurface Insights".

On the left side, there is a navigation menu with a "Learn" button and social media icons for LinkedIn and Email.

The main content area contains the following text and controls:

- CO₃²⁻ Concentration: 0.001 [m]
- If you have parameter sweeps enabled, the model below will show pH results for a range of CO₂ molalities. If sweeps are disabled it will only show results from the default starting value.
- Detailed explanation of the PFLOTRAN infile for this model is available in the Appendix (Opens in a new window)
- Interface Usage Instructions (Automatically opens in a new tab or window)

Below the text, there is a control panel for the model output file and parameters:

- Model output file: Carbonation_0D-obs-0.tec
- Parameter: "2-pH obs (1) (0.5 0.5 0.5)"
- Buttons: Download file, Add to graph, Graph all parameters, Clear graph, Change x axis to log scale, Change y axis to log scale, Manual scale, Toggle legend

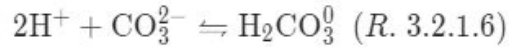
The graph shows a single data point at Time [y] = 0. The y-axis is labeled "2-pH obs (1) (0.5 0.5 0.5)" and ranges from 4.5 to 6. The x-axis is labeled "Time [y]" and ranges from -1 to 1.

Below the graph, there is a slider for "CO₃²⁻ molality" with a value of 0.001 and a "Use range" checkbox. The slider range is from 1e-4 to 0.1.

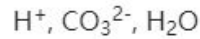
At the bottom, the model name is "Carbonation 0D" and there are "Run model" and "Hide menu" buttons.

Instantaneous equilibrium

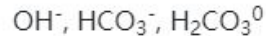
Aqueous Reactions:



Primary Species (our choice):



Secondary Species (our choice):



Model calculates value of different outputs

Only one value (model is 0d, 0-t)

Not very exciting -> but insightful

Parameter:

"2-pH obs (1) (0.5 0.5 0.5)"

"2-pH obs (1) (0.5 0.5 0.5)"

"3-Total H+ [m] obs (1) (0.5 0.5 0.5)"

"4-Total CO3-- [m] obs (1) (0.5 0.5 0.5)"

"5-Total H2O [m] obs (1) (0.5 0.5 0.5)"

"6-Free H+ [m] obs (1) (0.5 0.5 0.5)"

"7-Free CO3-- [m] obs (1) (0.5 0.5 0.5)"

"8-Free H2O [m] obs (1) (0.5 0.5 0.5)"

pH for CO₃⁻⁻ molality of 0.026

Interface Usage Instructions (Automatically opens in a new tab or window)

Model output file:

Carbonation_OD-obs-0.tec

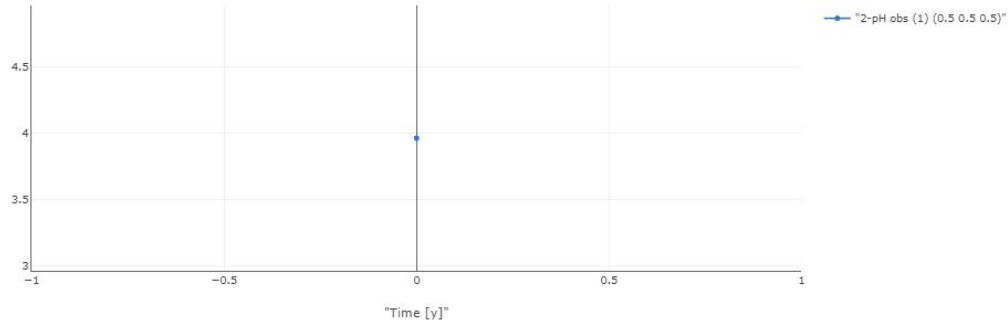
Parameter:

"2-pH obs (1) (0.5 0.5 0.5)"

Download file Add to graph Graph all parameters

Clear graph Change x axis to log scale

Change y axis to log scale Manual scale Toggle legend



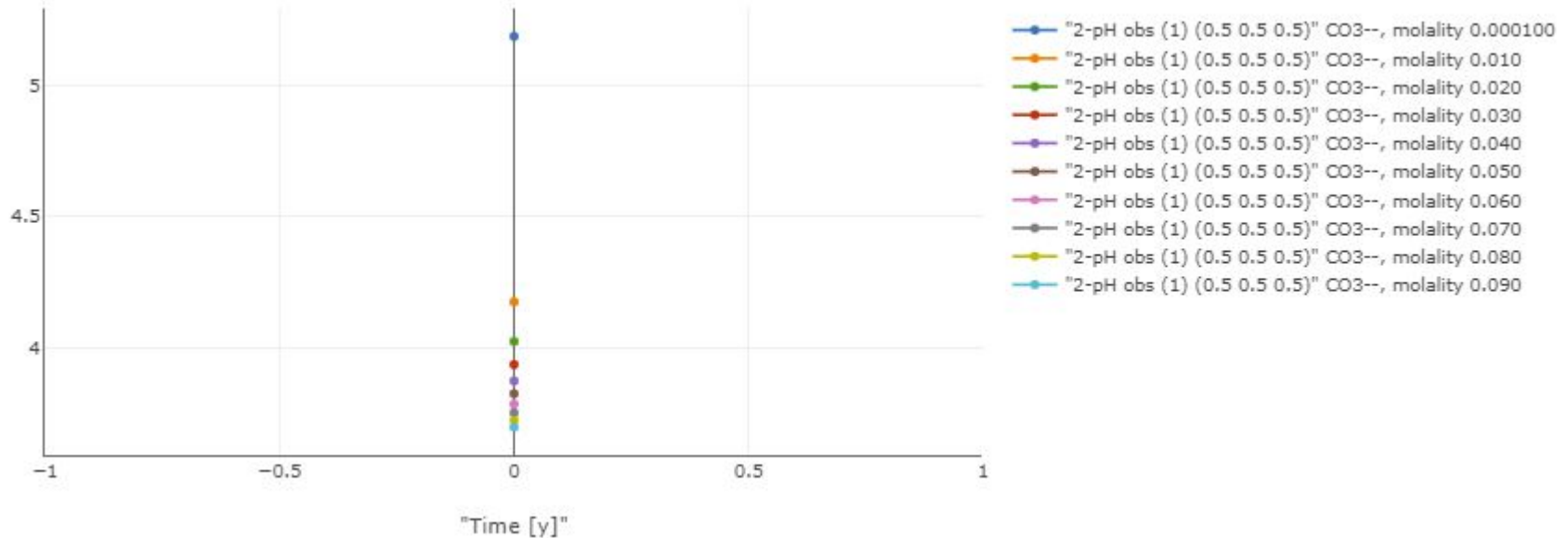
Model name: Carbonation OD

Run model Hide menu

We can also use range of molalities (model sweep)

Increase molality - decrease pH

Is what is expected



Example 2: movement of conservative tracer

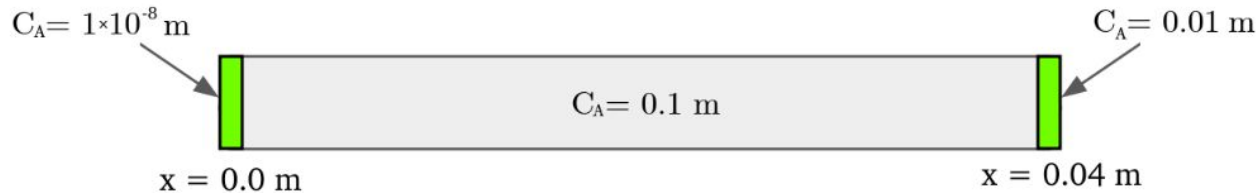
<https://learn.subsurfaceinsights.com/learn/#3.1.1.advection-&-dispersion>

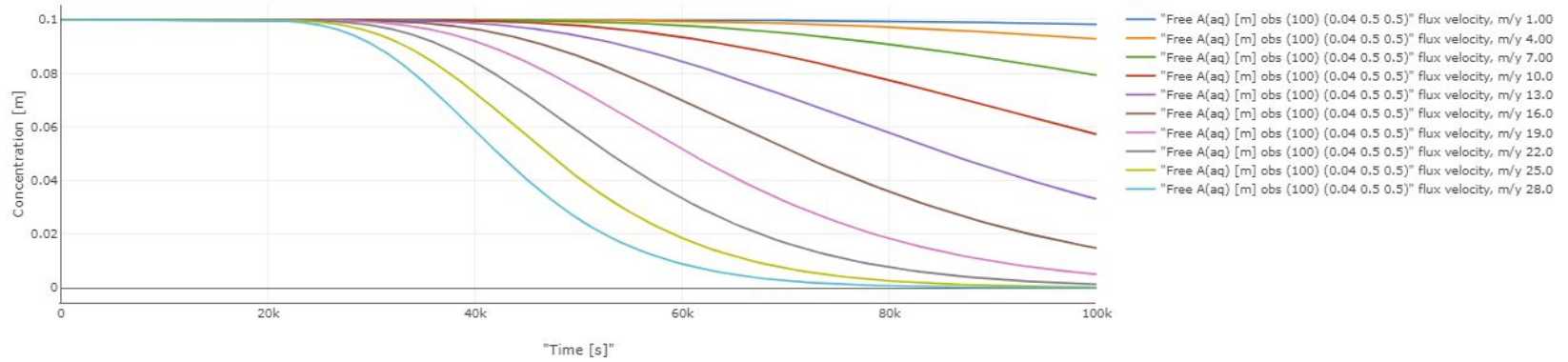
Introduction

This model simulates movement of a conservative tracer $A_{(aq)}$ in a horizontal column 0.04 m in length discretized into 100 grids with unit cross area. The initial concentration of tracer in the column is 0.1 m throughout. There are constant concentration boundaries at either end, set to 1×10^{-8} m at the left boundary ($x=0.0$ m) and 0.01 m at the right boundary ($x = 0.04$ m), as illustrated in Figure 4.2.2.1. The column 'fill' has the properties given in the table below:

Parameter	Value
Porosity*	1.0 [-]
Tortuosity	1.0 [-]
Rock Density	2800.0 [kg/m ³]
Specific Heat	1000.0 [J/(kg·K)]
Thermal Conductivity (wet)	0.5 [W/(K·m)]
Permeability	1.0×10^{-15} [m ²]

* Note that a porosity of 1.0 indicates the column is filled with fluid.





flux velocity, m/y

Use range

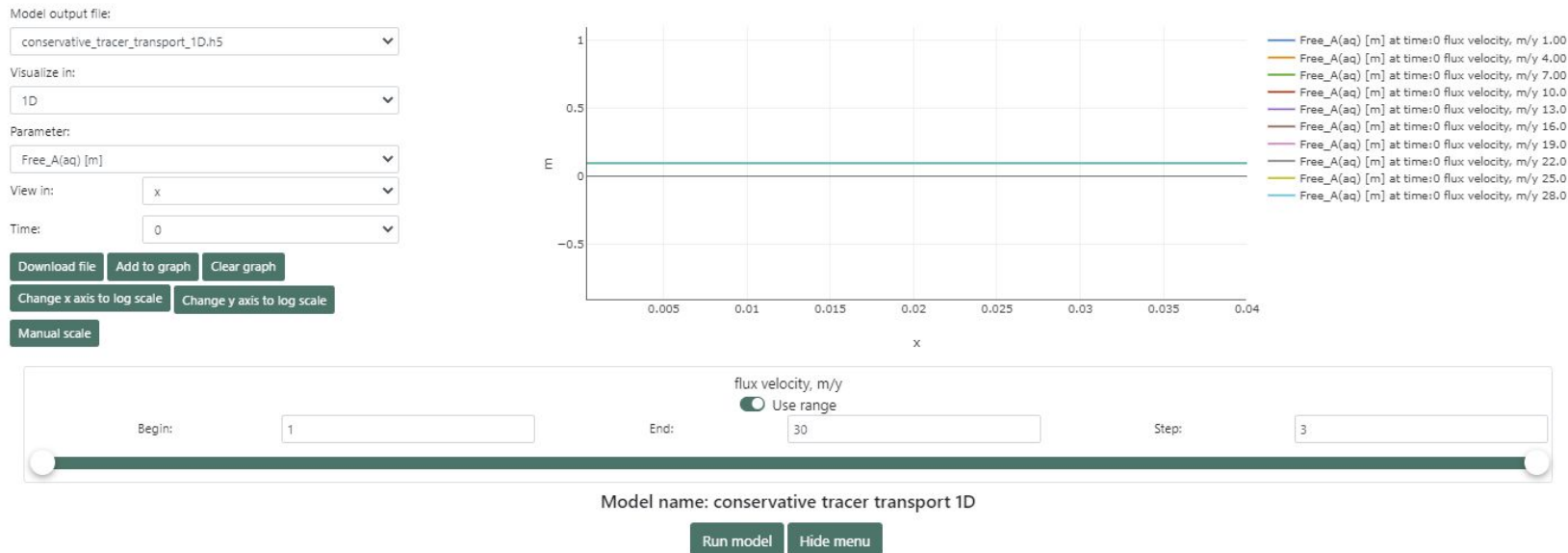
Begin: End: Step:

Model name: conservative tracer transport 1D

[Run model](#) [Show menu](#)

Model makes sense: as we increase the flux velocity, we will decrease the concentration quicker from the initial value of 0.1 M

Note that this is at one location in model, we look over time



Look at model at time 0: concentration is 0.1 M in all models (initial condition)

Interface Usage Instructions (Automatically opens in a new tab or window)

Model output file:

conservative_tracer_transport_1D.h5

Visualize in:

1D

Parameter:

Free_A(aq) [m]

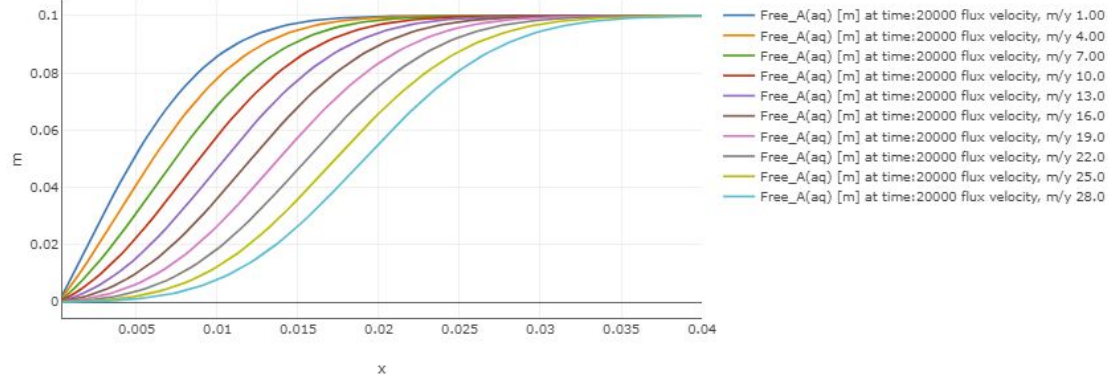
View in: x

Time: 20000

Download file Add to graph Clear graph

Change x axis to log scale Change y axis to log scale

Manual scale Toggle legend



flux velocity, m/y

Use range

Begin: 1

End: 30

Step: 3

Model name: conservative tracer transport 1D

Run model Hide menu

Look at model at time 20K : concentration changes as expected for different flux velocities

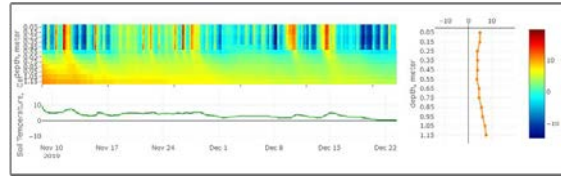
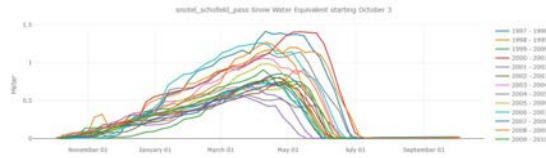
Course includes models of increasing complexity

- <https://learn.subsurfaceinsights.com/learn/#3.2.0.advection-dispersion-reaction-equation>
- <https://learn.subsurfaceinsights.com/learn/#5.1.3.example-3---acid-mine-drainage>
- + many more
- Allows users to experiment with parameters and get hands on understanding of modeling
- Provides incremental introduction to PFLOTRAN capabilities
- **Note 1:** Users can download PFLOTRAN files from interface for local modifications or analysis (note: PFLOTRAN v2)
- **Note 2:** dependent on demand model queue may be big - we will monitor this and add resources if needed

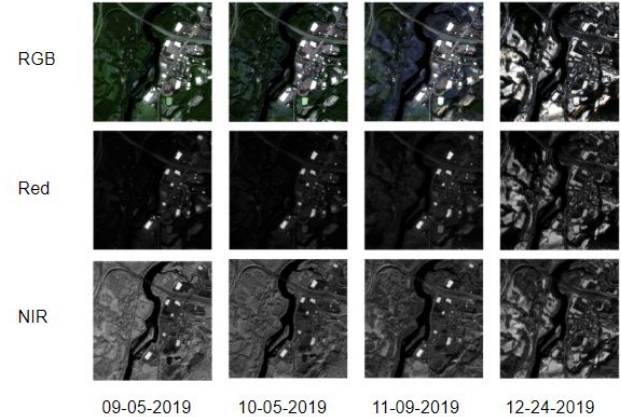
Data management, discovery and access mechanisms

- Reactive transport modeling needs more than just microbiological data
- Need easily accessible contextual data for microbial model building

- Soil temperature
- Elevation
- Soil moisture
- Solar radiation
- Vegetation cover
- Riverstage and flow
- Remote sensing data
- Snow thickness
- ...



Connecticut River (2 km x 2 km)



- Many data can be discovered through different APIs
- Contextual data use needs data normalization and integration in robust and scalable cyberinfrastructure - large part of Subsurface Insights focus

Cloud based PFLOTRAN and web based KBASE -
can we glue them together to create a microbial
modeling pipeline?



Cloud based PFLOTRAN and web based KBASE -
can we glue them together to create a microbial
modeling pipeline?



Turns out we can!

Nitrogen cycling – a case study



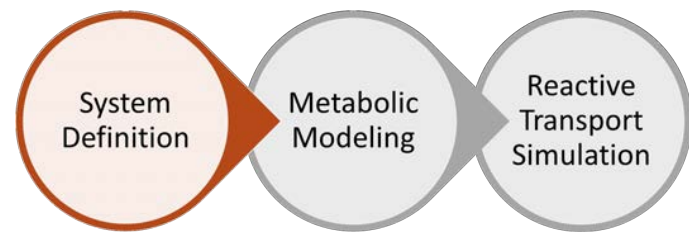
Hanford site river sediment
microbe-defined model
vs.
Literature-based model

(Graham et al., 2017; Graham et al. 2018)

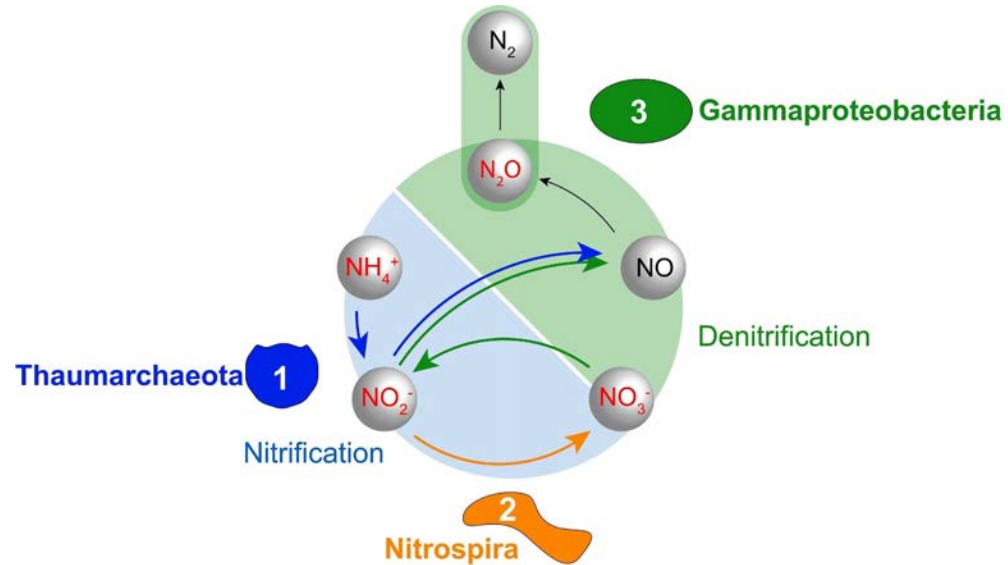
System Definition - Biology

Literature-based Model

- Generic 'Bugs'
 - Ammonium oxidizing bacteria
 - Nitrite oxidizing bacteria
 - Nitrate reducing bacteria



Site-specific Model



Multi-omics informed microbiology

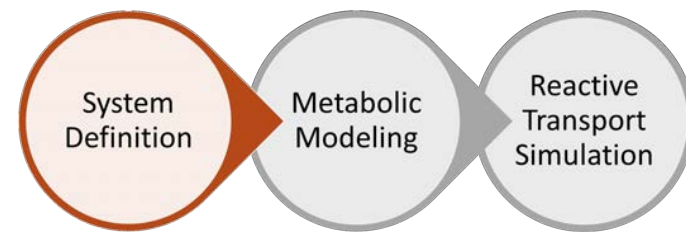
System Definition - Chemistry

Literature-based Model

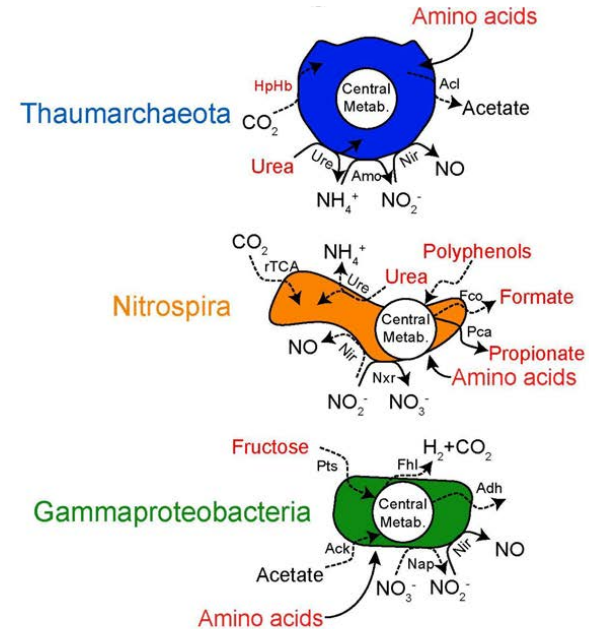
- Very limited chemistry

Process	Reactants	Products
Ammonium Oxidation	NH_4^+ , O_2 , CO_2 , HCO_3^-	H^+ , NO_2^-
Nitrite Oxidation	NO_2^- , NH_4^+ , O_2 , CO_2 , HCO_3^-	NO_3^-
Denitrification	NO_3^- , Acetate, H^+	HCO_3^- , CO_2 , N_2

(Liu & Wang, 2012)

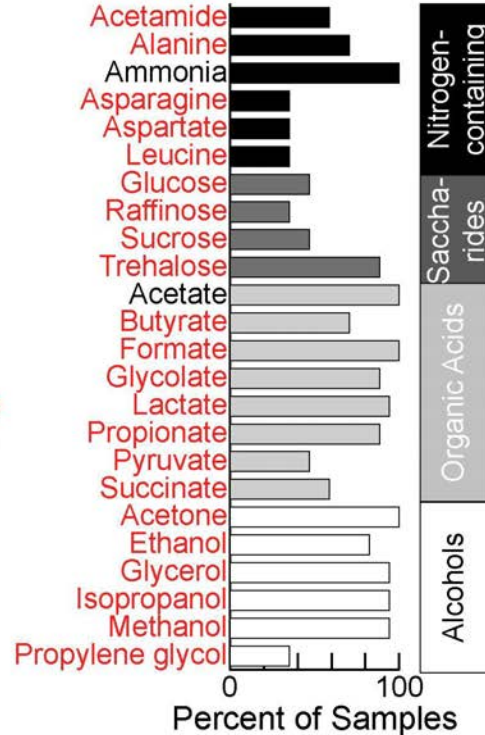
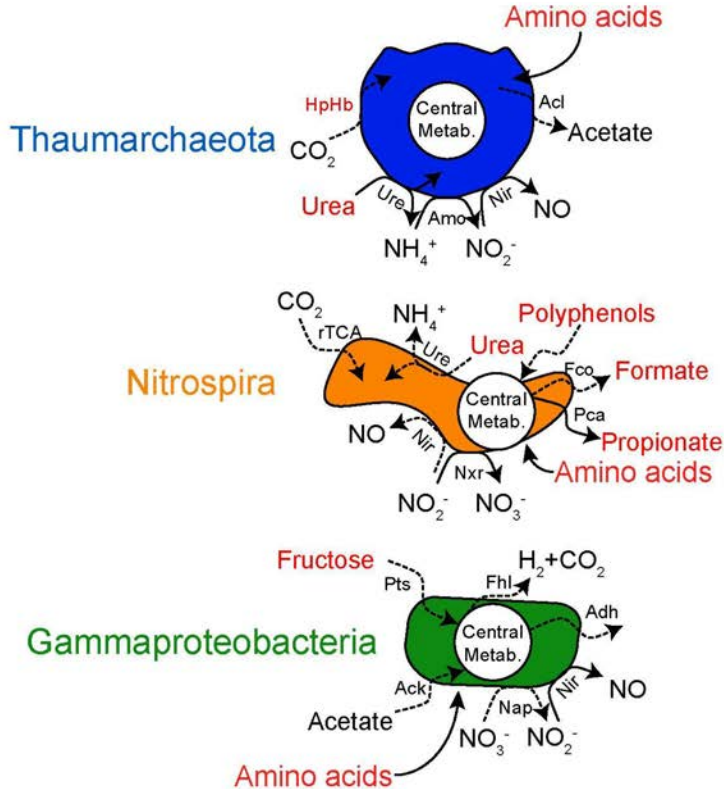
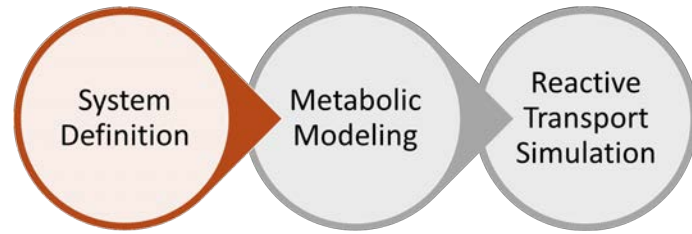


Site-specific Model



Theoretical **Multi-omics based**

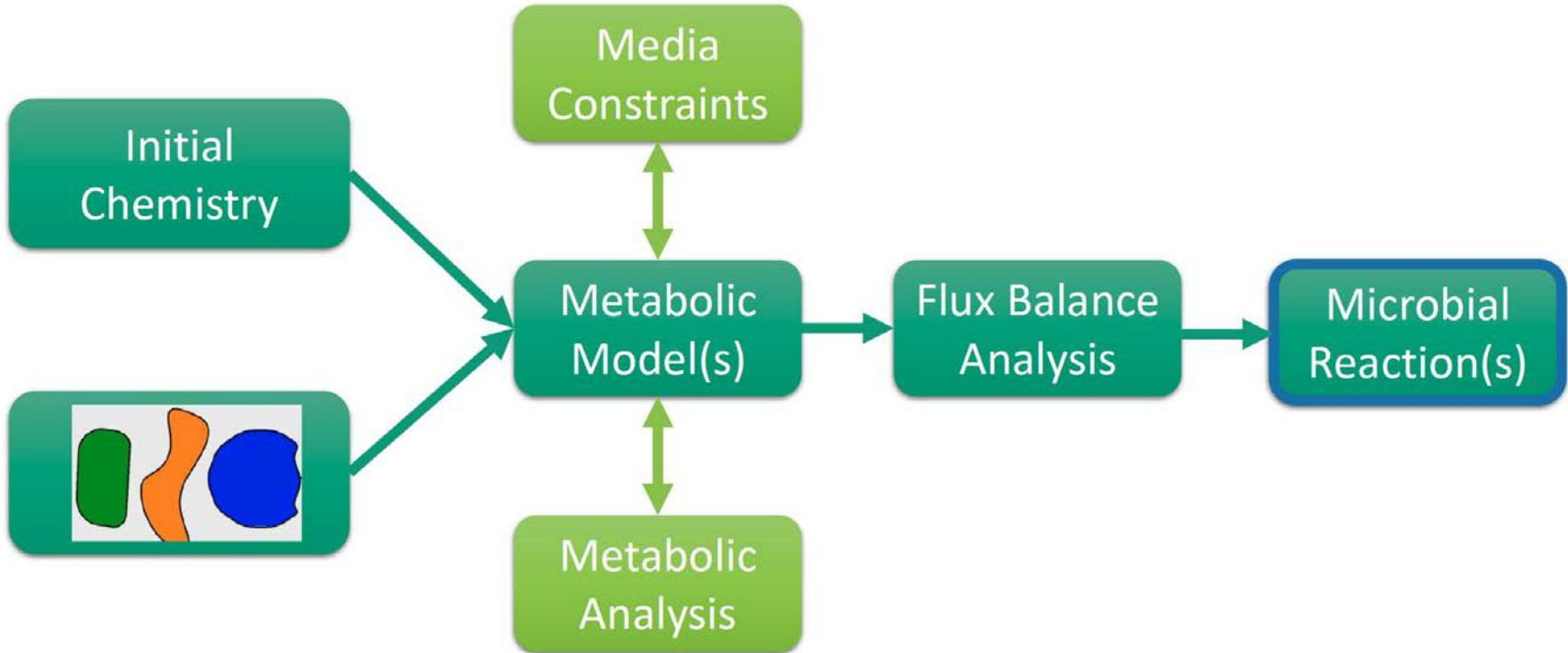
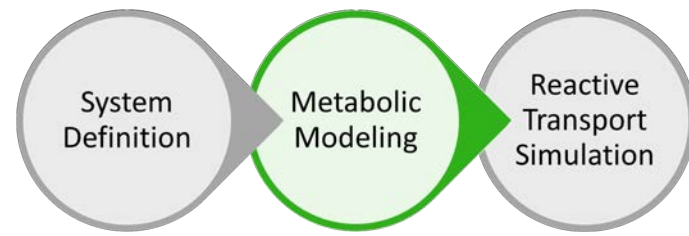
Multi-omics data identifies reaction scale processes



Theoretical reactions

Multi-omics defined reactions

Metabolic Modeling in KBase



Raw Output vs Processed

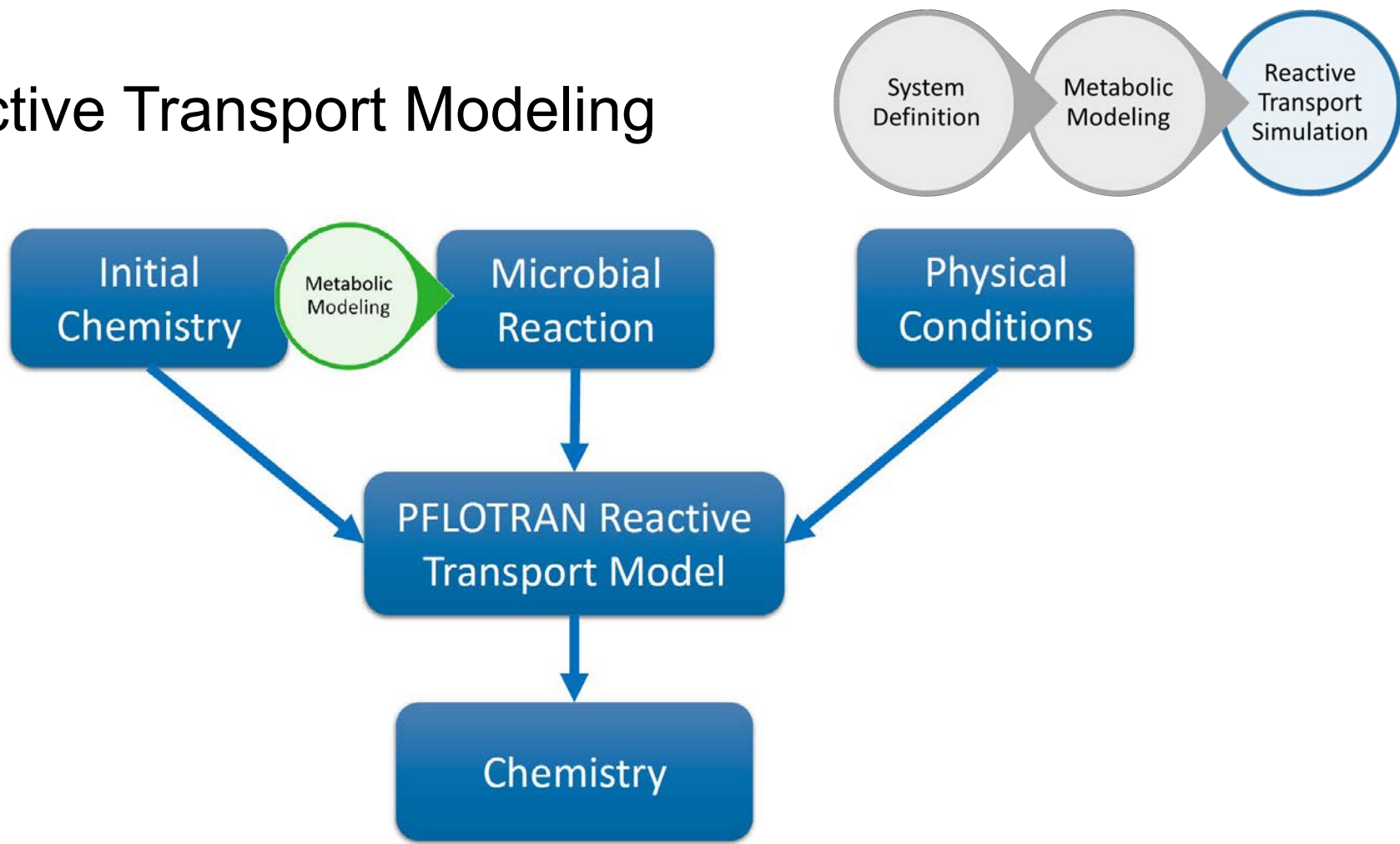
id	name	formula	charge	compartment	uptake	min_uptake	lowerbound	max_uptake	upperbound
1	cpd11576_e0	L-methionine	R-oxide_e0	CSH11N03S	0	0	0	-1000	0
2	cpd00001_e0	H2O_e0	H2O	0	-5.71458	-13.0953	-100	-3.26782	100
3	cpd00023_e0	L-Glutamate_e0	C5H8NO4	-1	0	-0.400642	-0.400642	-1000	-0.0400642
4	cpd00971_e0	Na+_e0	Na	1	0	0	-1000	0	0
5	cpd00058_e0	Cu2+_e0	Cu	2	0.000509282	5.09282e-05	-100	0.000509282	100
6	cpd00067_e0	H+_e0	H	1	9.15836	2.6499	-100	12	12
7	cpd00107_e0	L-Leucine_e0	C6H13NO2	0	0	0	-2.23682	-1000	0
8	cpd00013_e0	NH3_e0	H4N	1	0	0	0	0	0
9	cpd00060_e0	L-Methionine_e0	C5H11NO2S	0	0	0	-1000	0	0
10	cpd00322_e0	L-Isoleucine_e0	C6H13NO2	0	0	0	-2.23682	-1000	0
11	cpd00637_e0	D-Methionine_e0	C5H11NO2S	0	0	0	-1000	0	0
12	cpd00035_e0	L-Alanine_e0	C3H7NO2	0	0	-3.81891	-1000	0	0
13	cpd01092_e0	Allantoin_e0	C4H5N4O3	-1	0	0	-1000	0	0
14	cpd00117_e0	D-Alanine_e0	C3H7NO2	0	-1.93638	-3.81891	-1000	0	0
15	cpd00307_e0	Cytosine_e0	C4H5N3O	0	0	0	-1000	0	0
16	cpd00254_e0	Mg_e0	Mg	2	0.000509282	5.09282e-05	-100	0.000509282	100
17	cpd00159_e0	L-Lactate_e0	C3H5O3	-1	0	0	-1000	0	0
18	cpd10516_e0	fe3_e0	Fe	3	0.00203713	0.000203713	-100	0.00203713	100
19	cpd01914_e0	L-Methionine	S-oxide_e0	CSH11N03S	0	0	0	-1000	0
20	cpd00162_e0	Aminoethanol_e0	C2H8NO	1	0	0	-1000	0	0
21	cpd00007_e0	O2_e0	O2	0	0	0	0	0	0
22	cpd00156_e0	L-Valine_e0	C5H11NO2	0	0	0	-2.65622	-1000	0
23	cpd00011_e0	CO2_e0	CO2	0	-0.01	-8.79294	-100	-0.01	0
24	cpd00099_e0	Cl-_e0	Cl	-1	0.000509282	5.09282e-05	-100	0.000509282	100
25	cpd00149_e0	Co2+_e0	Co	2	0.000509282	5.09282e-05	-100	0.000509282	100
26	cpd00528_e0	N2_e0	N2	0	-3.12635	-4.90945	-100	-3	-3
27	cpd00030_e0	Mn2+_e0	Mn	2	0.000509282	5.09282e-05	-100	0.000509282	100
28	cpd00209_e0	Nitrate_e0	NO3	-1	10	6.18109	10	10	10
29	cpd00048_e0	Sulfate_e0	O4S	-2	0.0365994	0.00365994	0	0.0365994	10
30	cpd00029_e0	Acetate_e0	C2H3O2	-1	15	4.37511	15	15	15
31	cpd00009_e0	Phosphate_e0	HO4P	-2	0.133547	0.0133547	-100	0.133547	100
32	cpd00034_e0	Zn2+_e0	Zn	2	0.000509282	5.09282e-05	-100	0.000509282	100
33	cpd00242_e0	H2CO3_e0	CH3O	-1	-15.7029	-17.1596	-100	-1	-1
34	cpd00205_e0	K+_e0	K	1	0.000509282	5.09282e-05	-100	0.000509282	100
35	cpd00063_e0	Ca2+_e0	Ca	2	0.000509282	5.09282e-05	-100	0.000509282	100
36	cpd11416_c0	Biomass_c0	null	0	-0.164472	-0.164472	-1000	-0.0164472	0

```

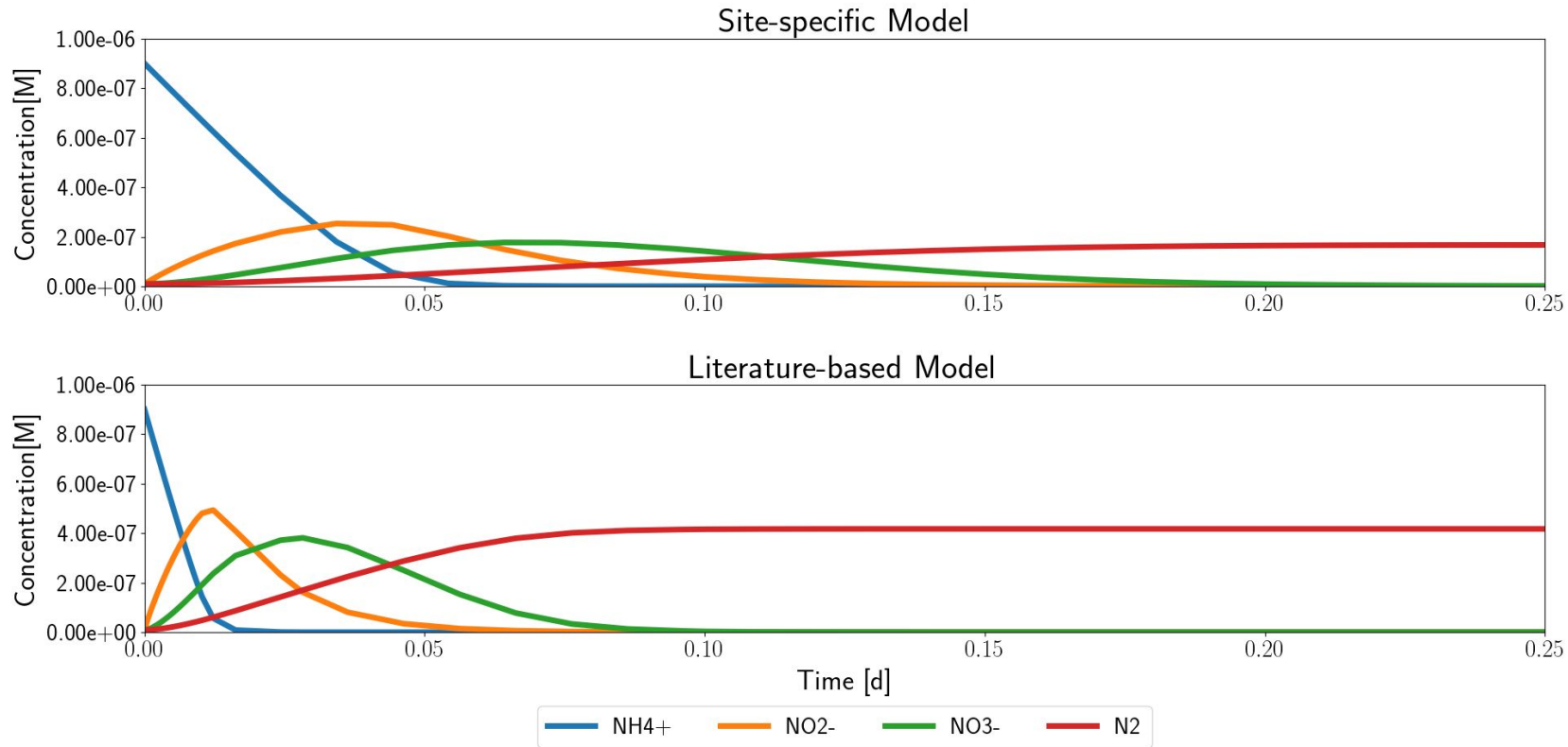
1 NiteStep1
2 1 biomass compounds omitted from reaction string
3 10.0 NH4+ + 0.000765313 Mg++ + 0.00306125 Fe+++ + 0.000765313 Co++ + 1.31783 O2(aq)
  + 0.000765313 Zn++ + 9.73097 HCO3- + 0.000765313 Mn++ + 0.054999 SO4-- +
  0.000765313 Cu++ + 0.200688 HPO4-- + 0.000765313 Ca++ + 0.000765313 Cl- +
  0.000765313 K+ -> 7.22562 H+ + 7.88192 NO2-
4 YIELD 0.247157
5
6
7 Denite
8 1 biomass compounds omitted from reaction string
9 0.000508709 Cu++ + 9.14819 H+ + 0.000508709 Mg++ + 0.00203483 Fe+++ + 0.133397
  HPO4-- + 0.0365582 SO4-- + 0.000508709 Mn++ + 0.000508709 Ca++ + 0.000508709 Co++ +
  0.000508709 K+ + 0.000508709 Zn++ + 15.0 Acetate- + 0.000508709 Cl- + 10.0 NO3- ->
  0.400191 LGlutamate- + 1.93945 DAlanine(aq) + 3.12583 N2(aq) + 15.7133 HCO3-
10 YIELD 0.164287
11
12
13 NiteStep2
14 1 biomass compounds omitted from reaction string
15 10.0 NO2- + 0.00032004 Cu++ + 1.0 NH4+ + 0.00032004 Mg++ + 0.00128016 Fe+++ +
  4.06889 HCO3- + 0.00032004 Ca++ + 0.00032004 K+ + 0.0839232 HPO4-- + 0.0229996
  SO4-- + 0.00032004 Mn++ + 0.00032004 Co++ + 0.00032004 Zn++ + 0.00032004 Cl- ->
  10.1138 NO3-
16 YIELD 0.103357
17
18
19 Ncycle.NS1
20 Reaction does not proceed
21

```

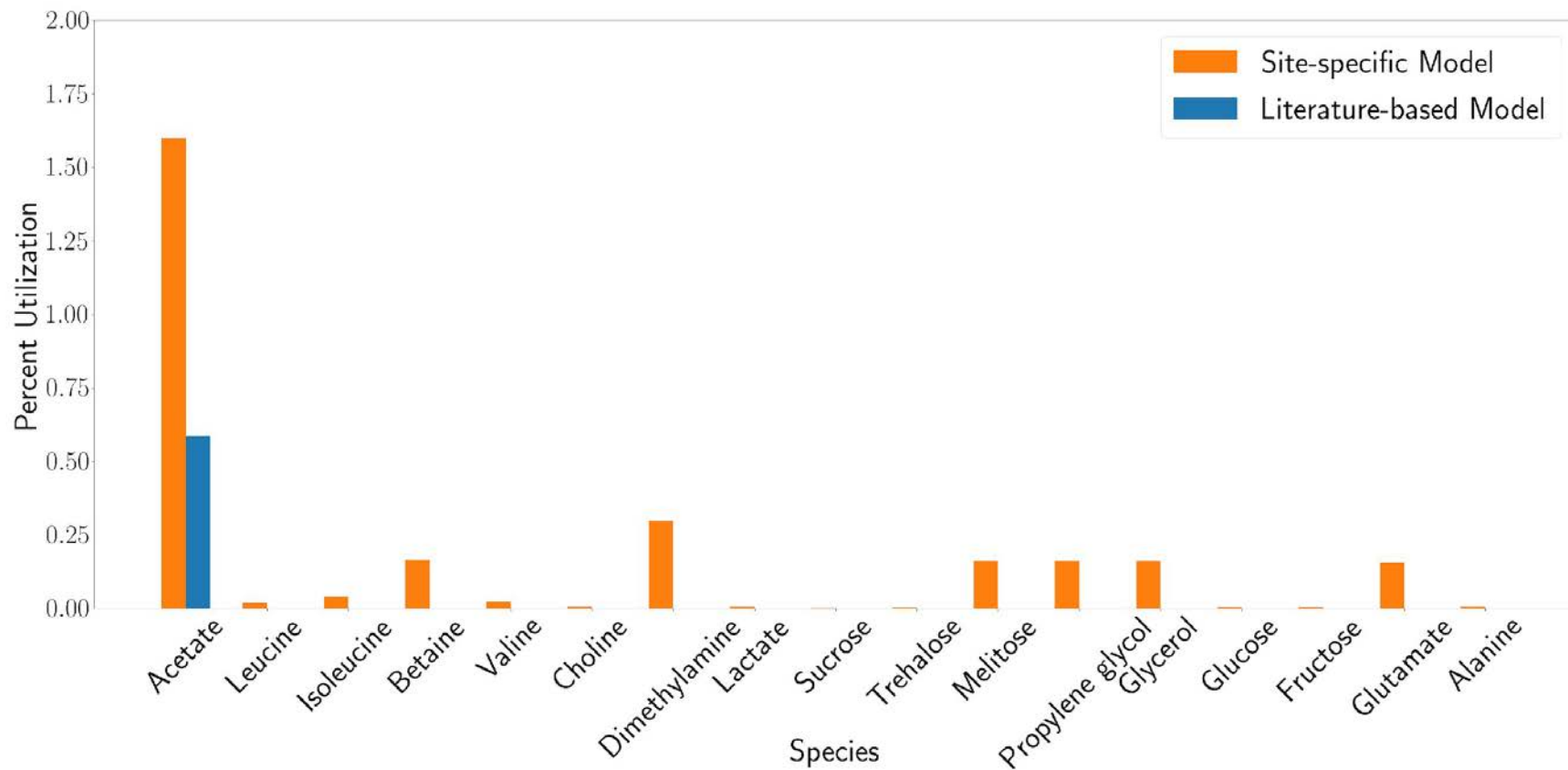
Reactive Transport Modeling



High level agreement, difference in details



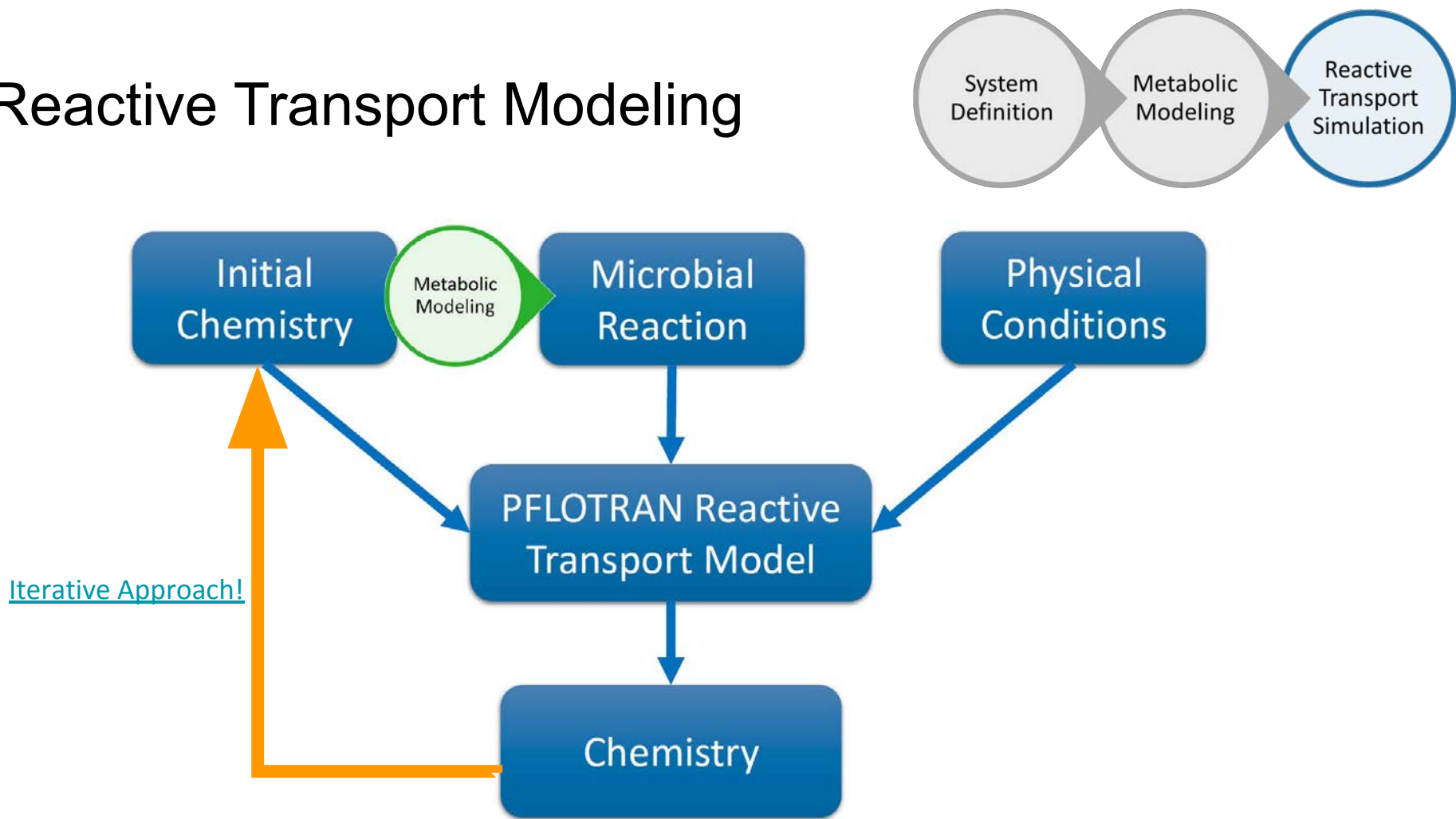
Site-specific models account for site-specific chemistry and conditions



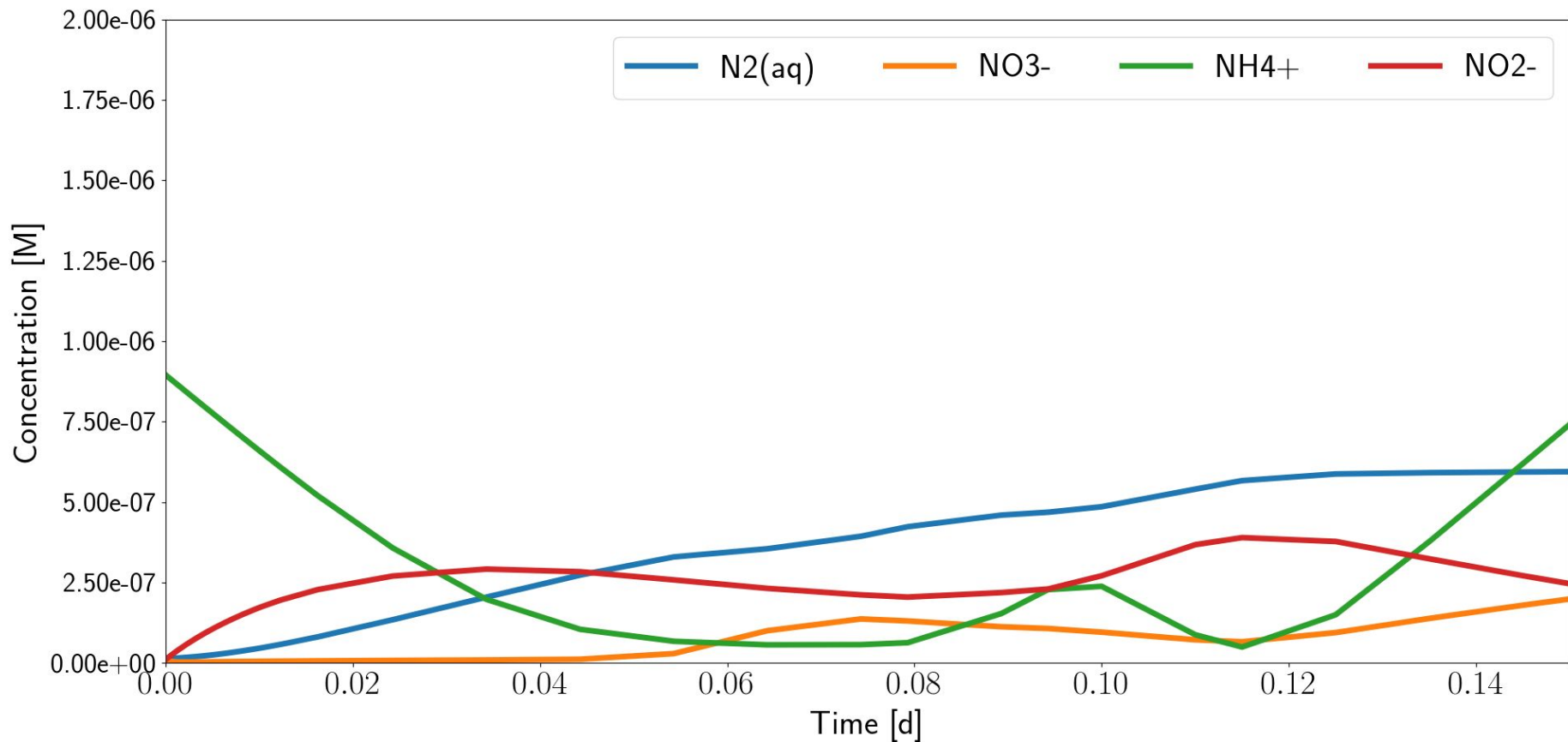
Live Example

<https://pflotranmodeling.paf.subsurfaceinsights.com/pflotran-simple-model/>

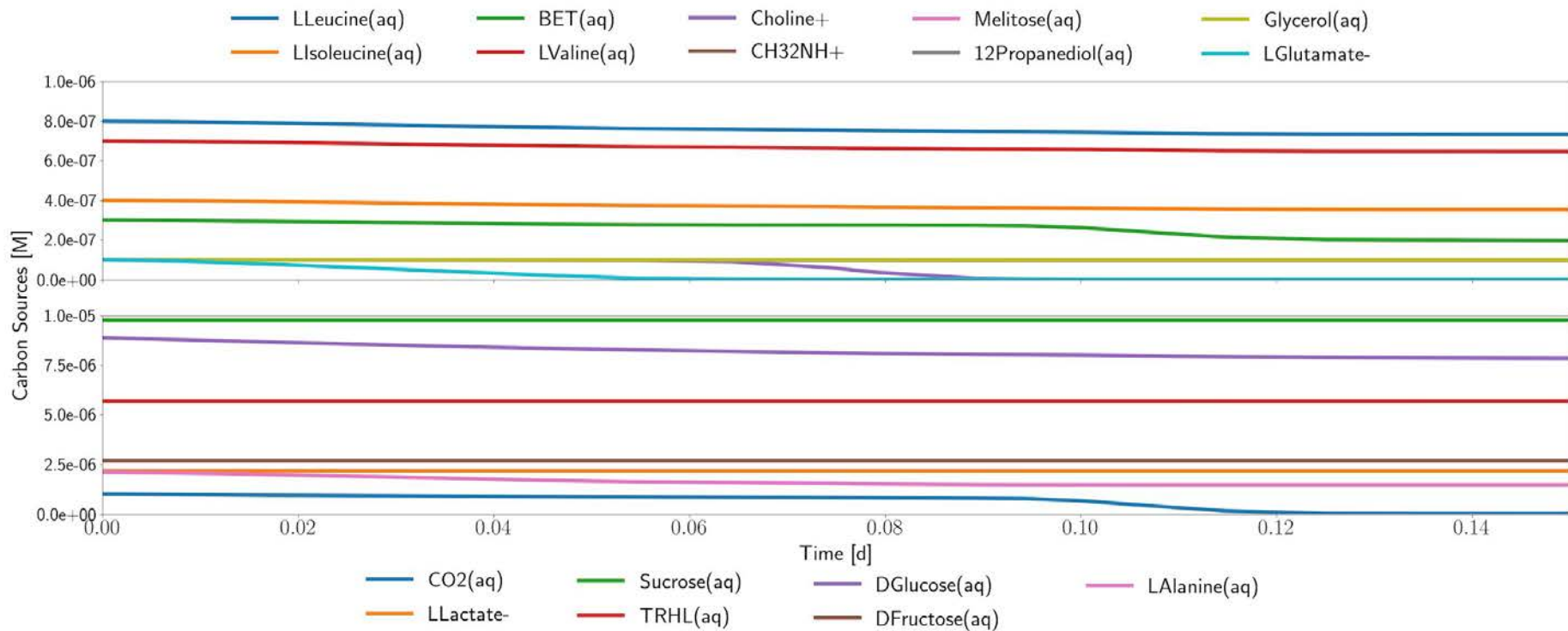
Reactive Transport Modeling



Continuous Operation



Sequential Carbon Source Switching



Summary

- Online course should make attendees familiar with modeling basics
- A robust cyberinfrastructure will make your life easier
- KBase - PFLOTRAN pipeline allows for comprehensive modeling of subsurface microbiology

Contact Rebecca or Roelof for further details