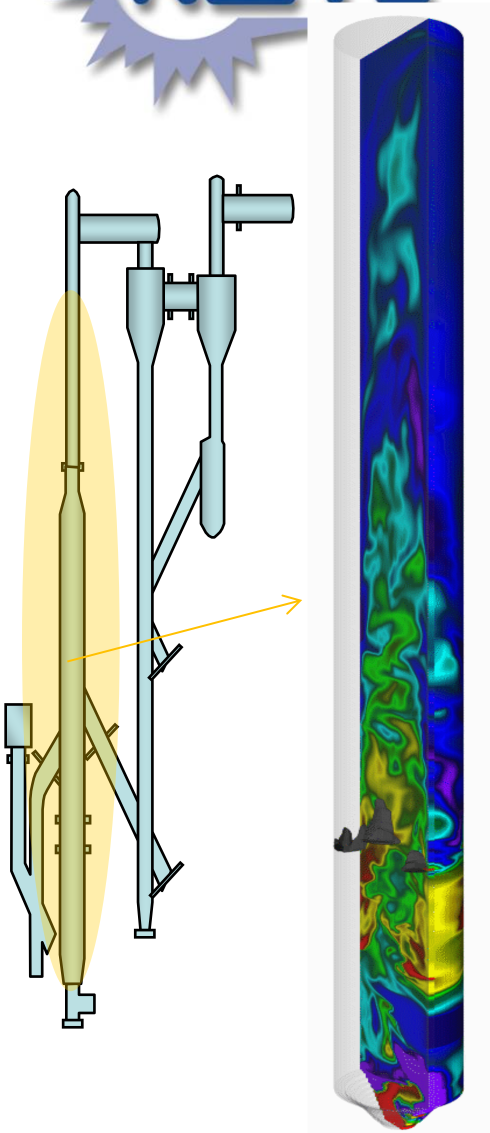
NATIONAL ENERGY TECHNOLOGY LABORATORY



Advanced Chemical Modeling Through Surrogate Response Models and Uncertainty Quantification in C3M

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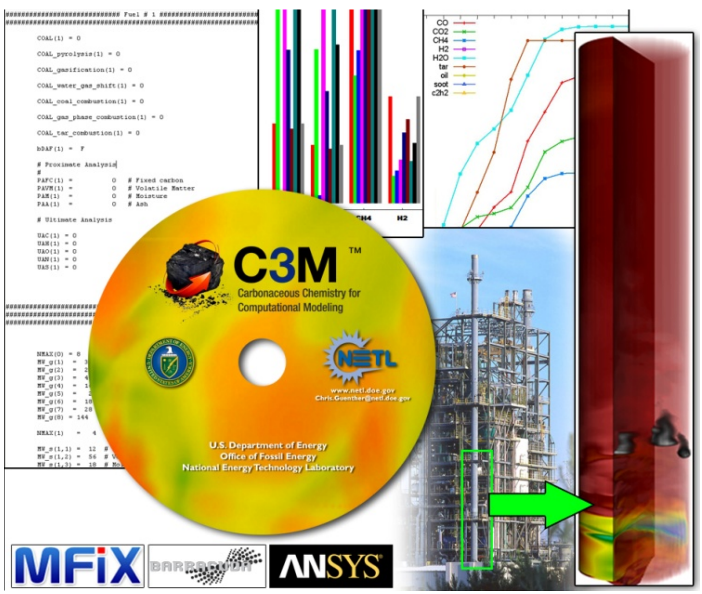
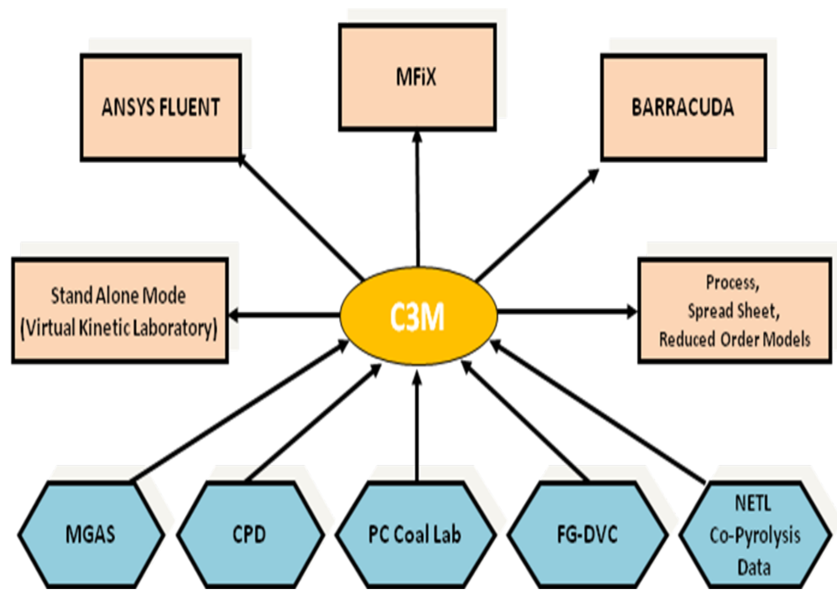
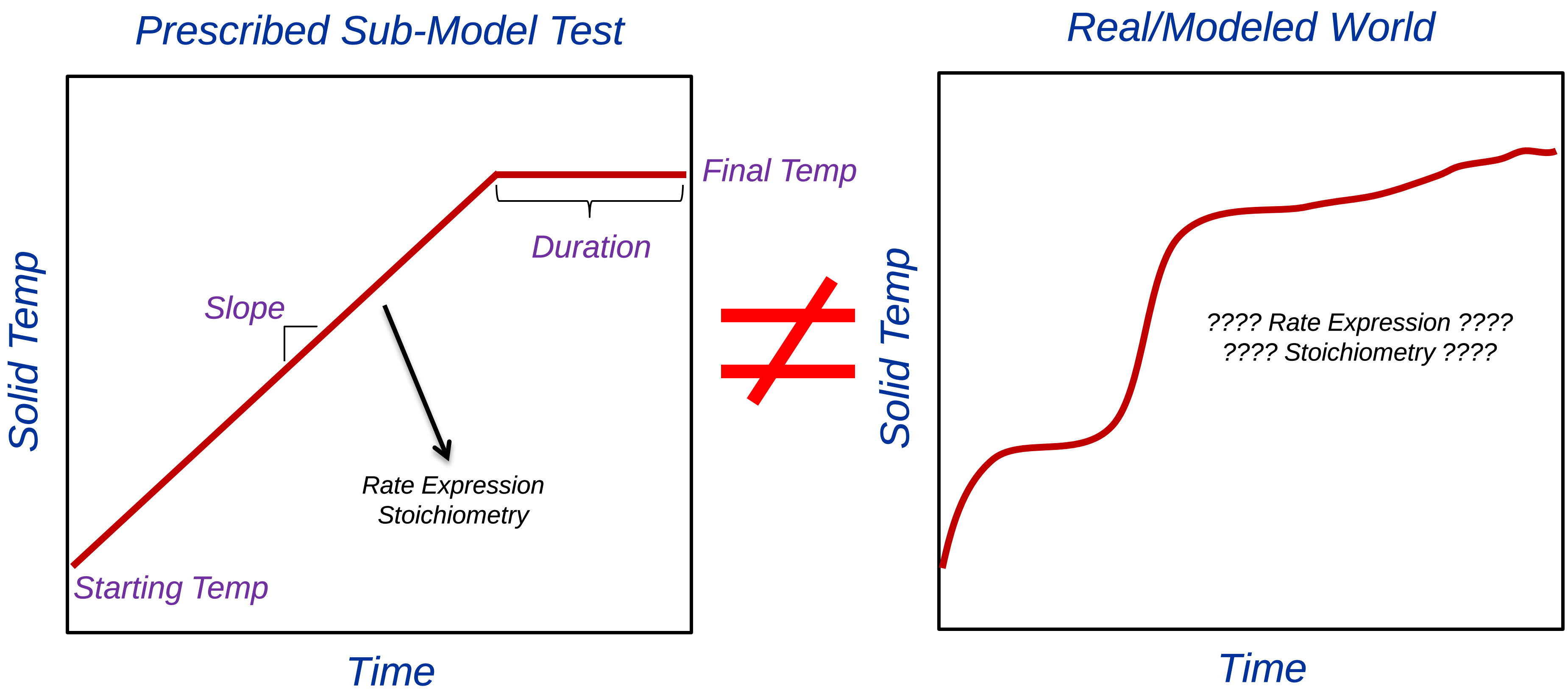
What is C3M

- **Chemical Kinetics Management Software**
  - Provide a user friendly, comprehensive interface between reliable sources of kinetic data and reacting, multi-phase CFD models
  - Provide “Virtual Kinetic Laboratory” for quickly assessing the validity of a chemical equation sets before going to full scale, expensive models
  - Manage all formatting and units for code specific implementation
  - Provide information for other computational models





Motivation

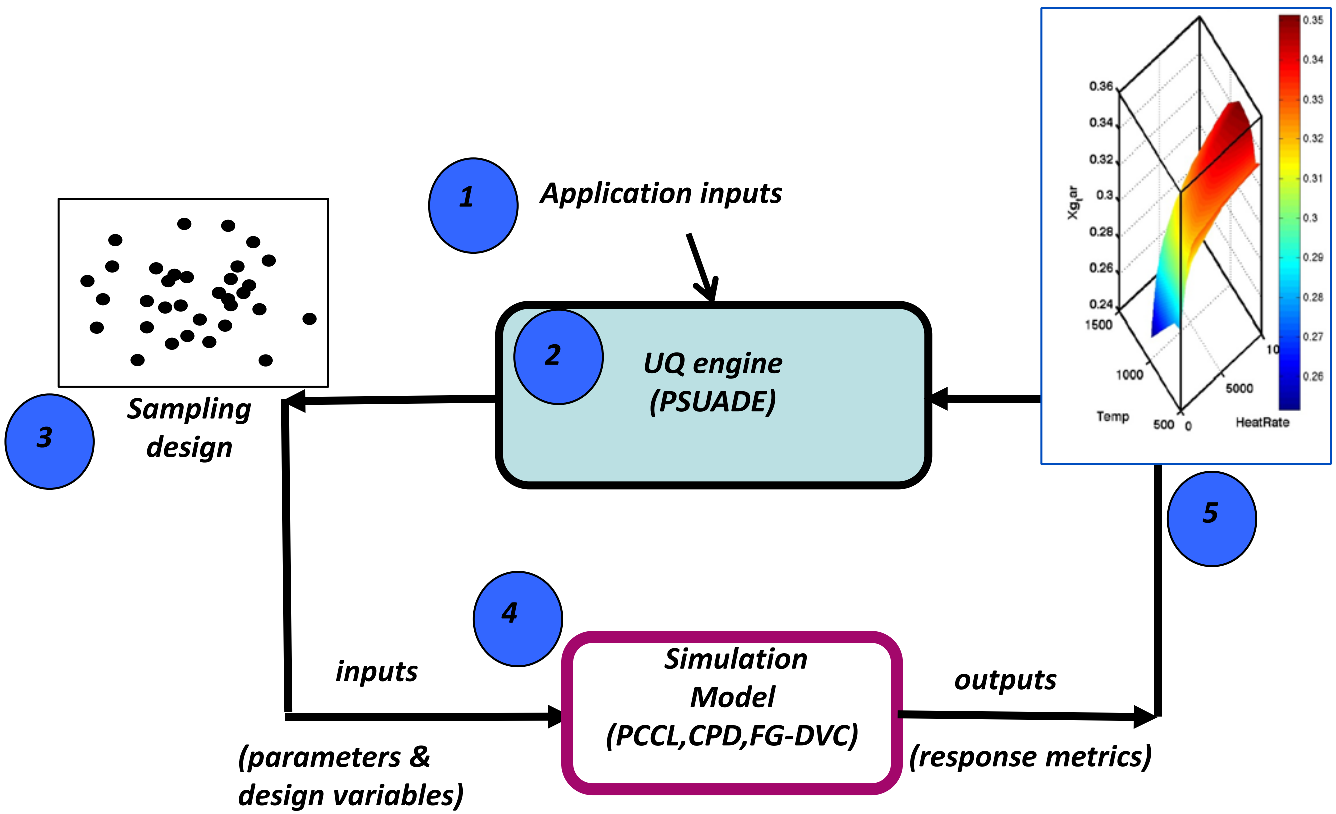


- **Current Focus: Devolatilization**
  – Uncertainty in Heating and Final Temp

Solution: Use Tools from UQ

Uncertainty Quantification

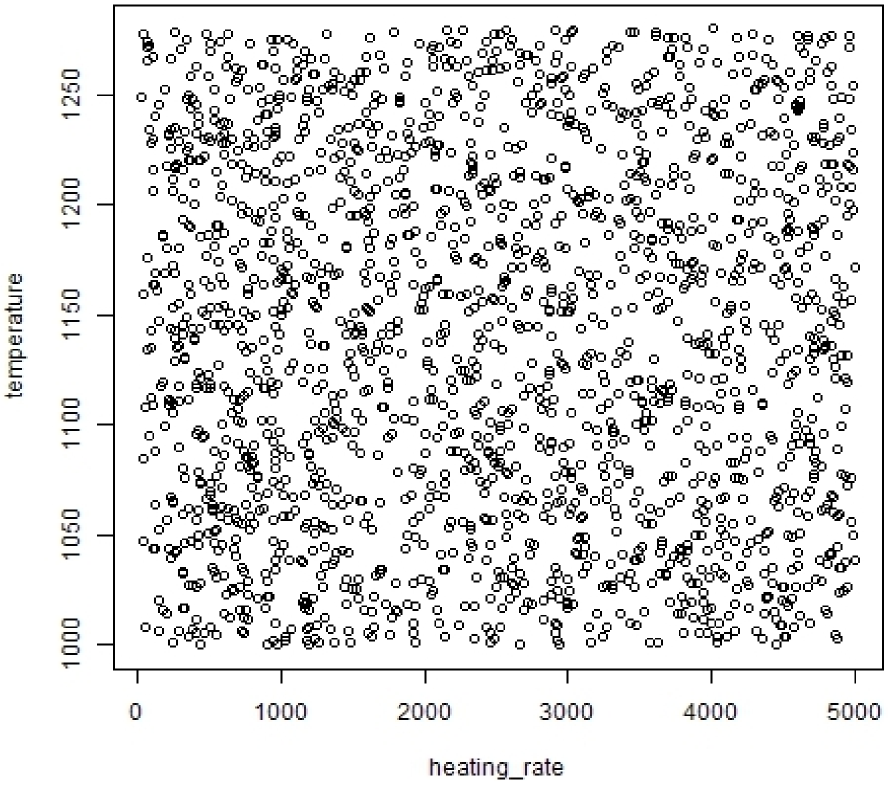
Input Uncertainty Propagation and Quantification (Non-intrusive method)



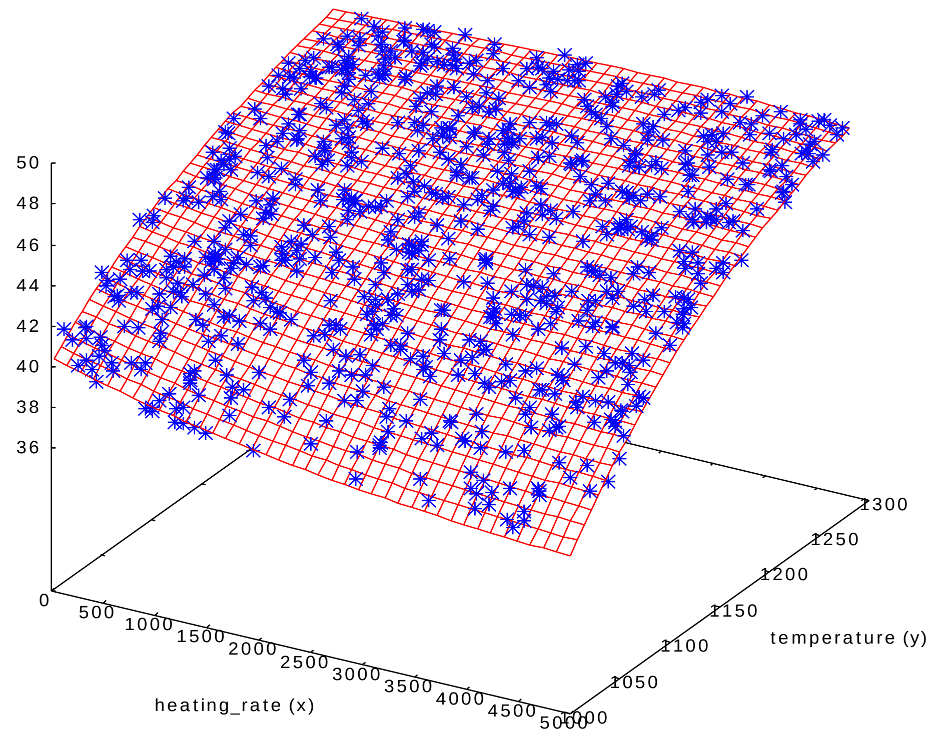
Solution: Use Tools from UQ

Uncertainty Quantification
PCCL with PRB Example

Sample Design Space

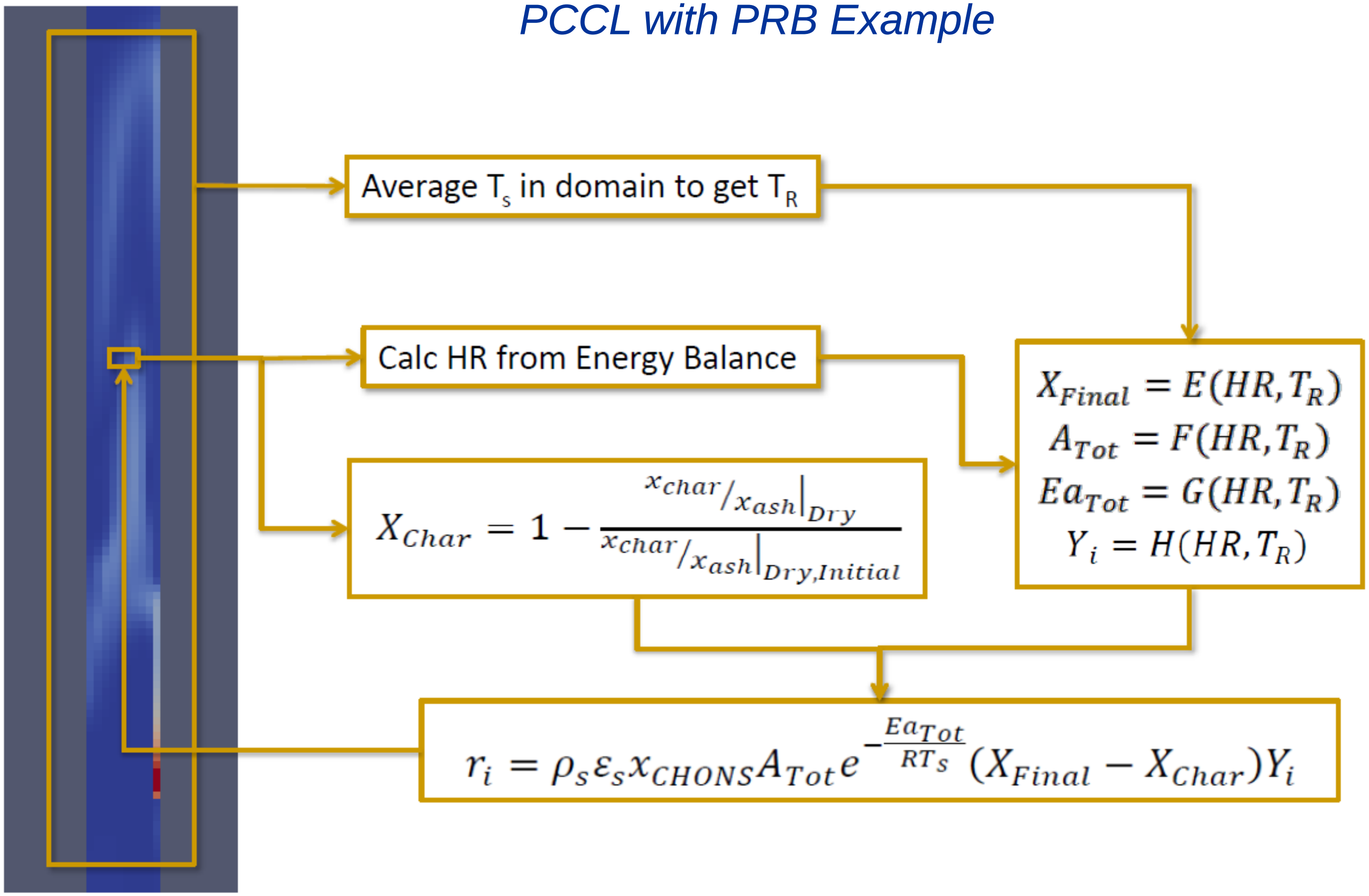


Example Response Surface
Total Volatile Yield



Solution: Use Tools from UQ

Build Surrogate Model in CFD
PCCL with PRB Example

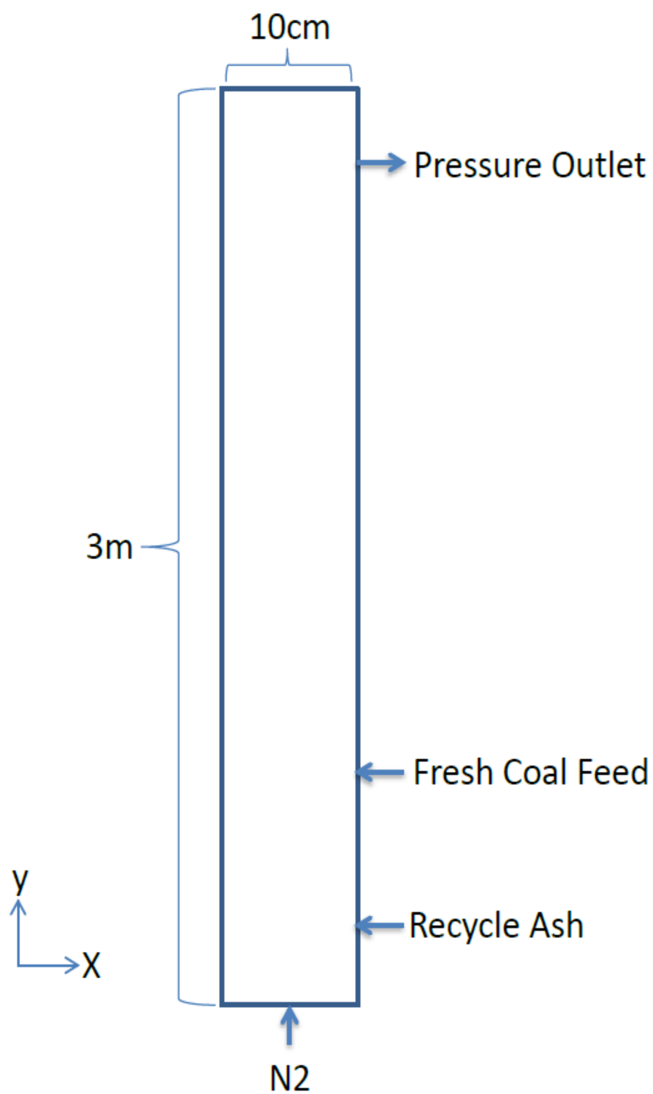


7 component coal model: Ash Moisture, Carbon, Hydrogen, Oxygen, Nitrogen, Sulfur
Each gas formed during devolatilization has it's own chemical formula and rate:

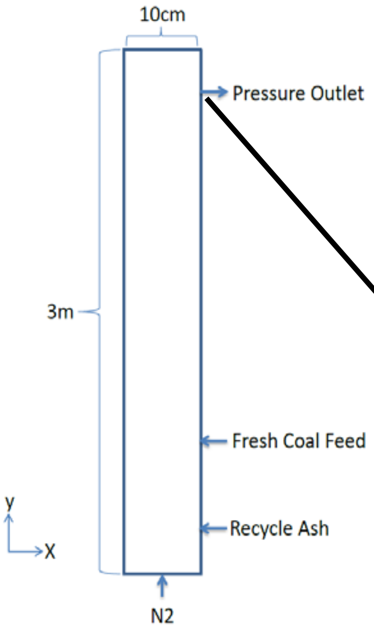
$$\alpha C_c + \beta C_H + \gamma C_O + \delta C_N + \varepsilon C_S \rightarrow C_\alpha H_\beta O_\gamma N_\delta S_\varepsilon$$

Example Test Case

Pseudo 2D Transport Reactor

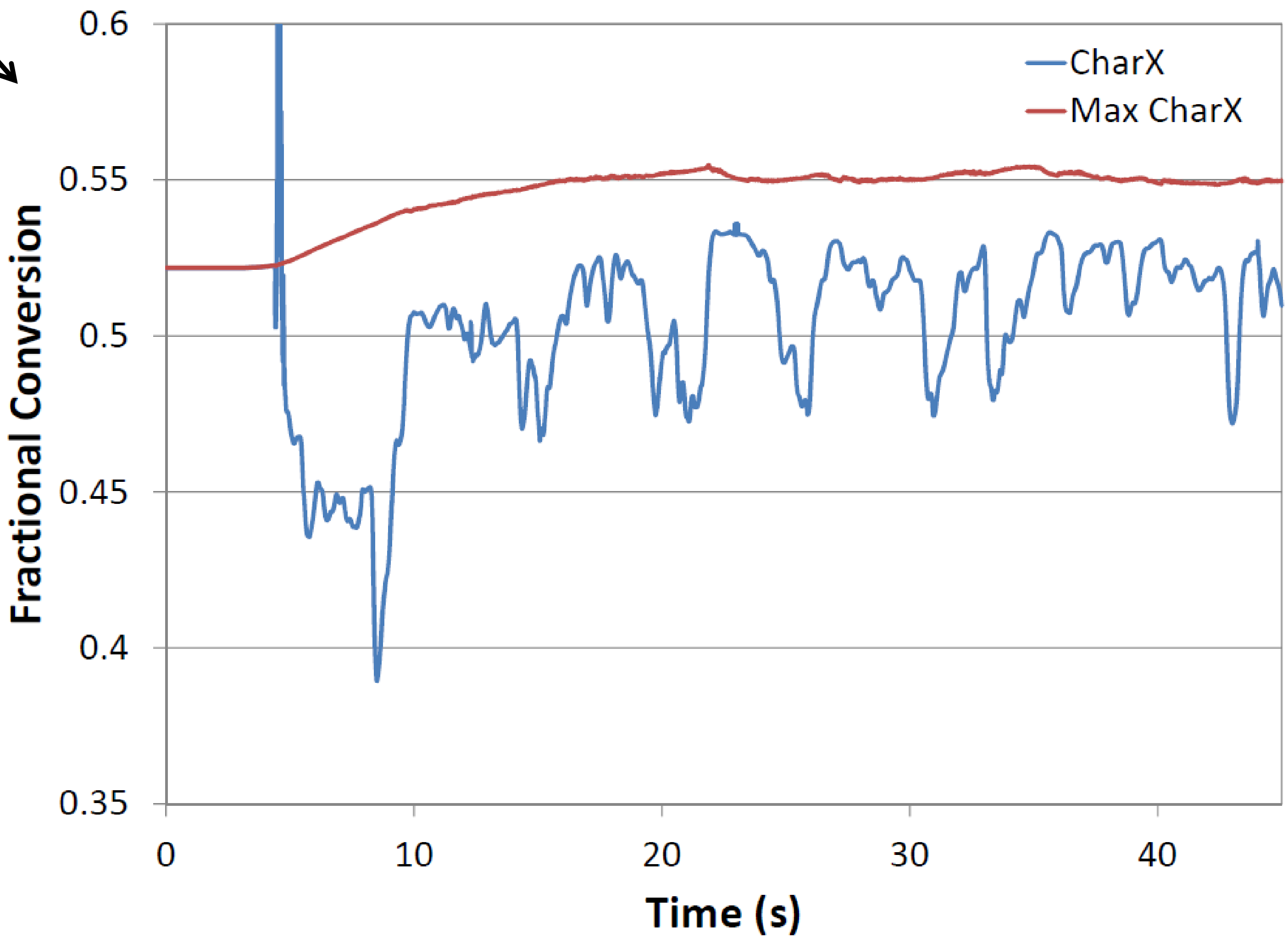


- **Grid: 10 x 320 (~1cm res)**
- **N_2/Recycle at 1280K**
- **Outlet Pressure 1.55 Mpa**
- **PRB injected at 298K, 0.1g/s**
- **Heats of Reaction Calculated**
- **Tr estimated from solids temp at outlet**

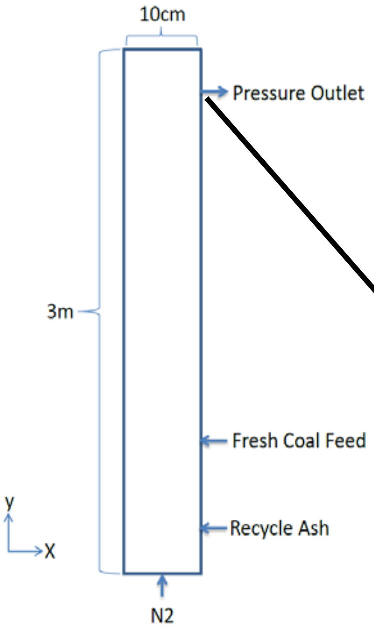


Example Test Case

Coal Conversion at Exit

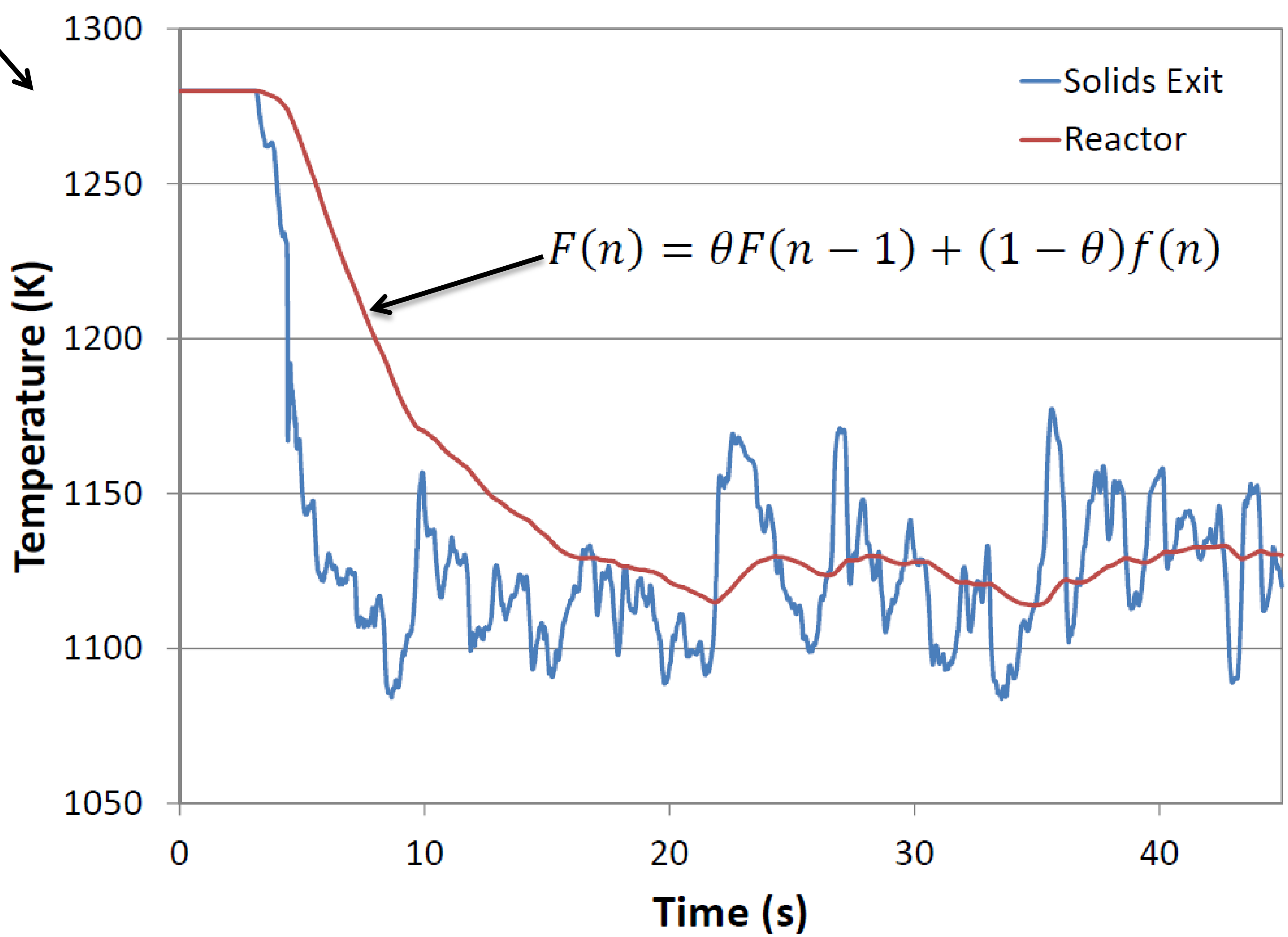


The coal conversion at the outlet is high and relatively closely follows the trends in the maximum conversion predicted by PCCL



Example Test Case

Solids and Reactor Temperature at Exit

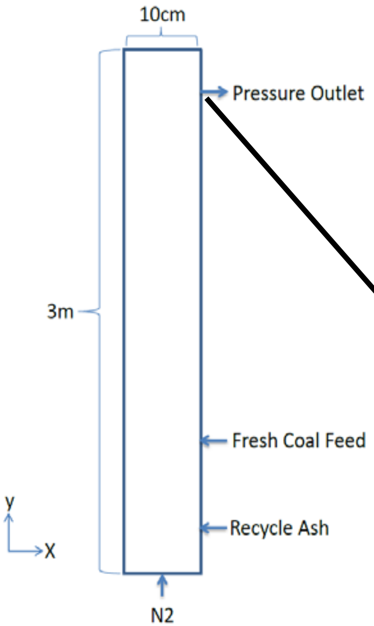


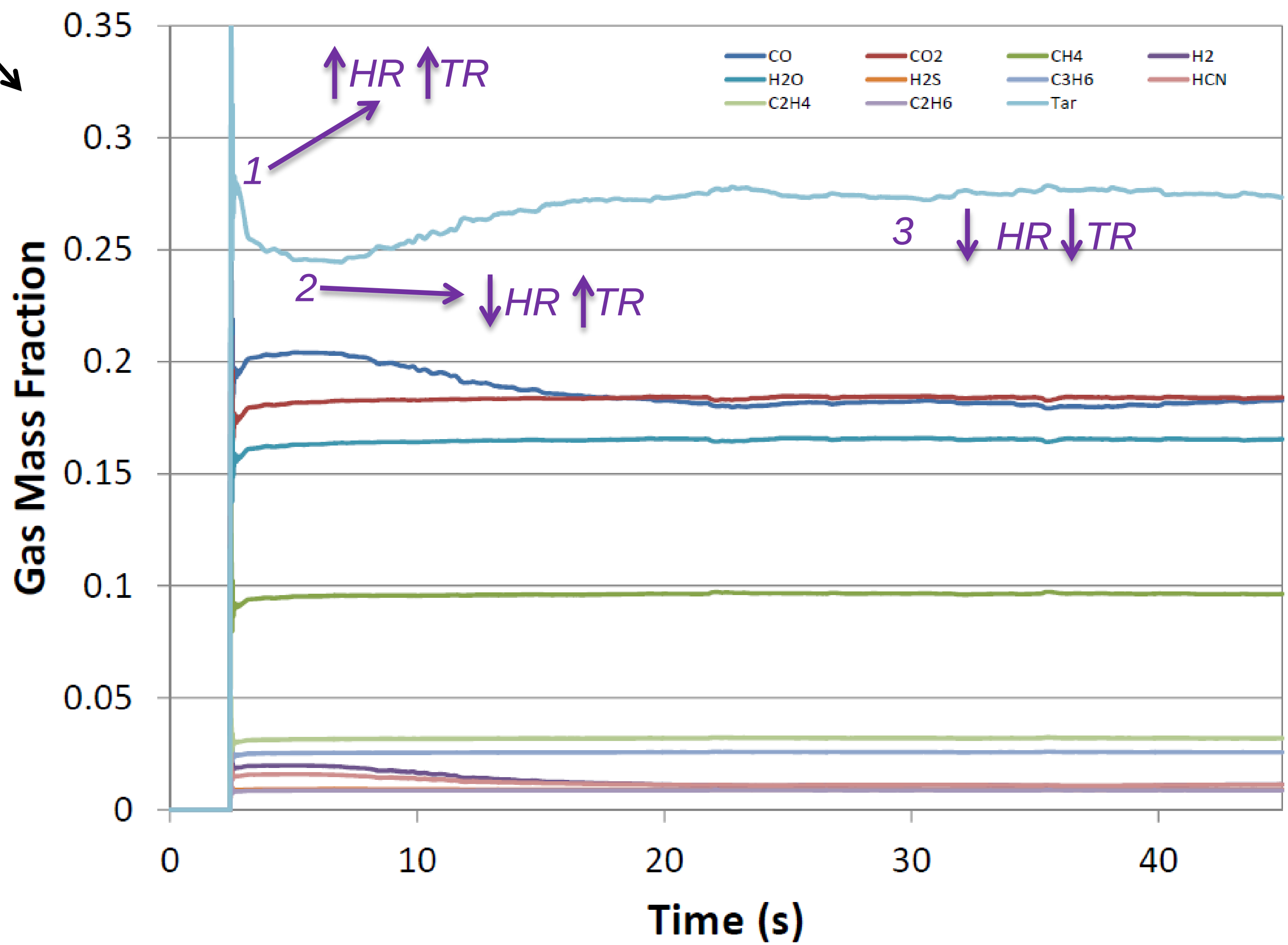
Reactor temp. is calculated by time filtering the solids temp. at the exit of the reactor

Solids take 3-5s to move from inlet to outlet

Example Test Case

Fractional Product Yield, Mass Basis at exit

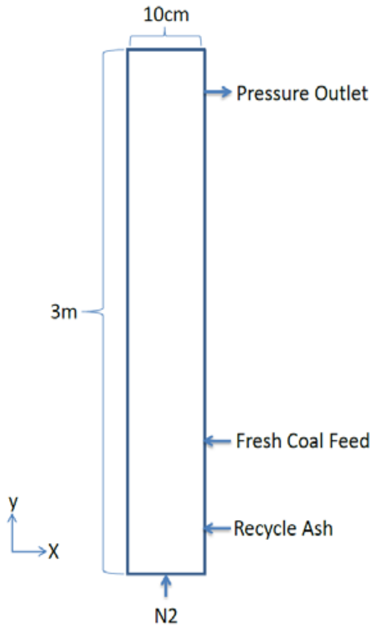




Initial heating rate is very high, and calculated reactor temp is high

Heating rate falls quickly as solids cool the path to travel

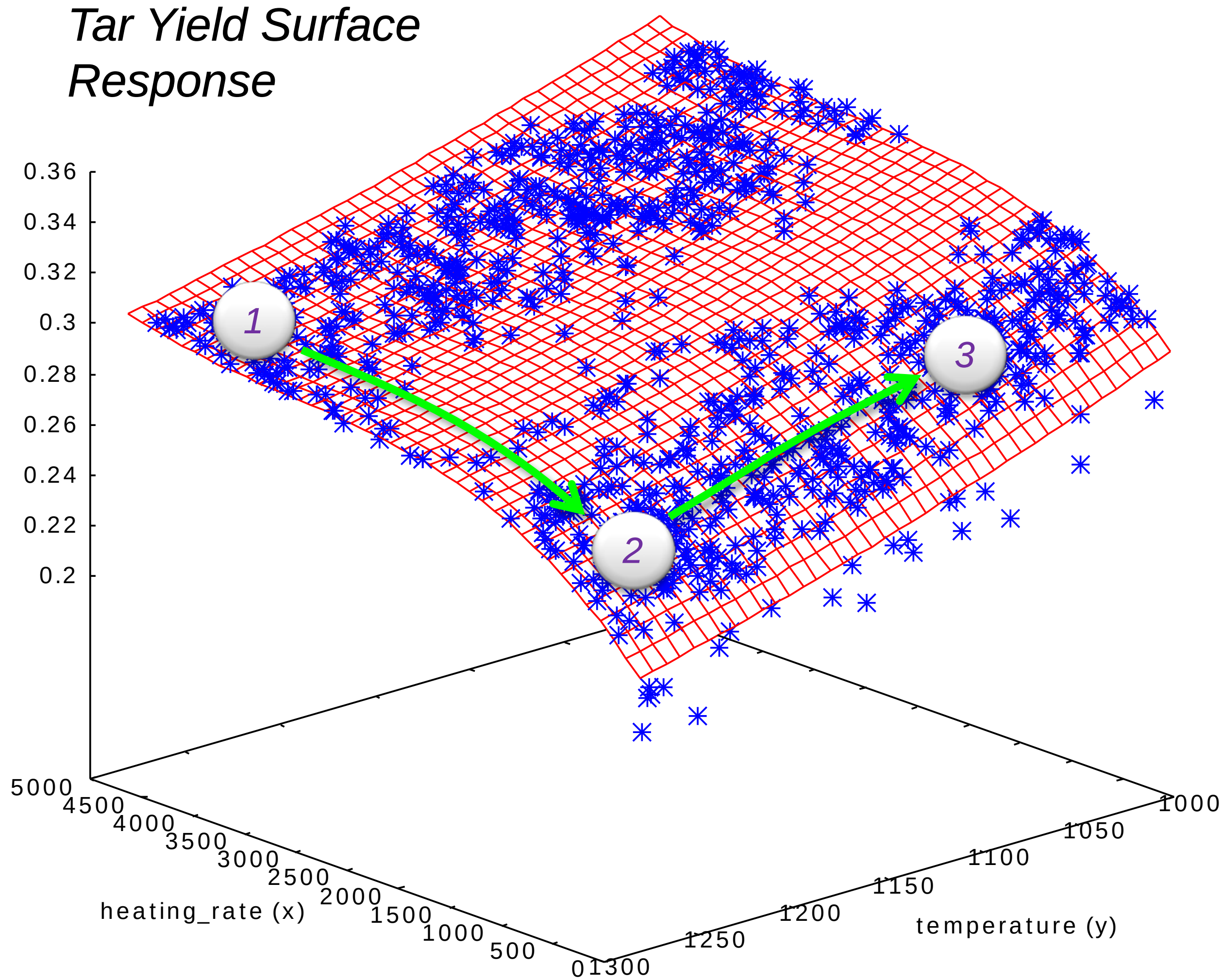
Cooler solids exit reactor and begin to set the reactor temp



Example Test Case

Understanding Product Yields

Tar Yield Surface Response



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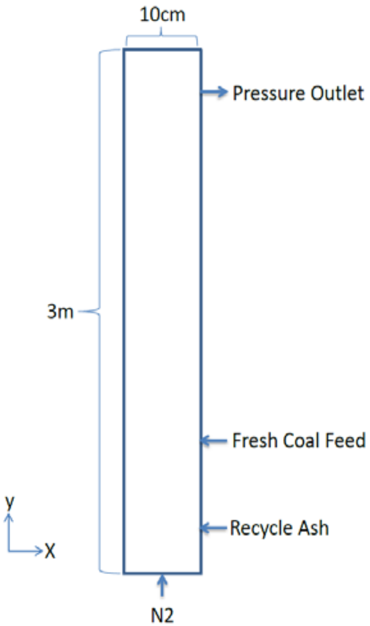
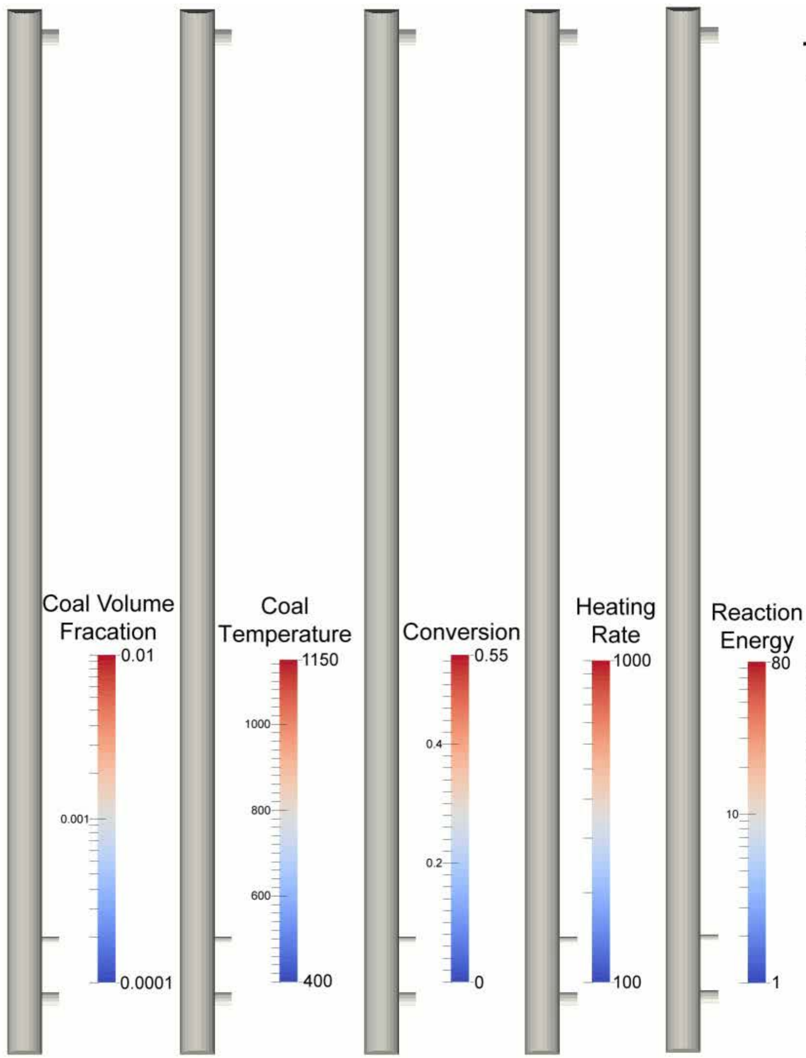
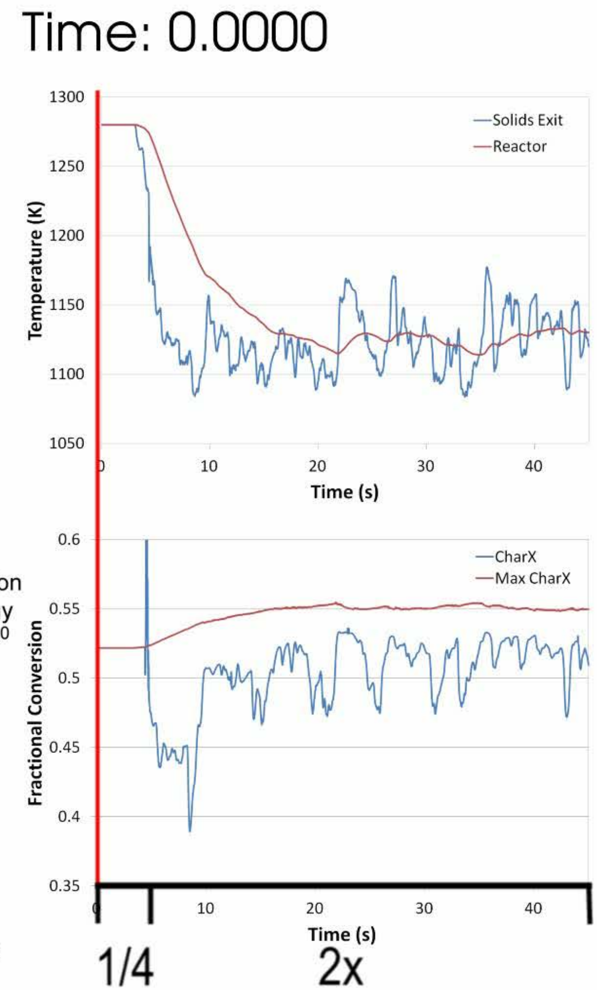


Example Test Case

Understanding Product Yields





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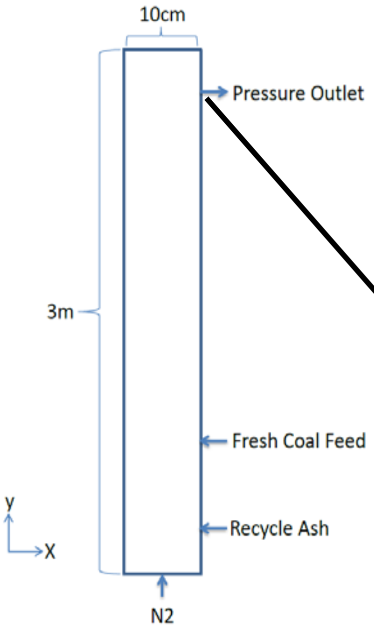
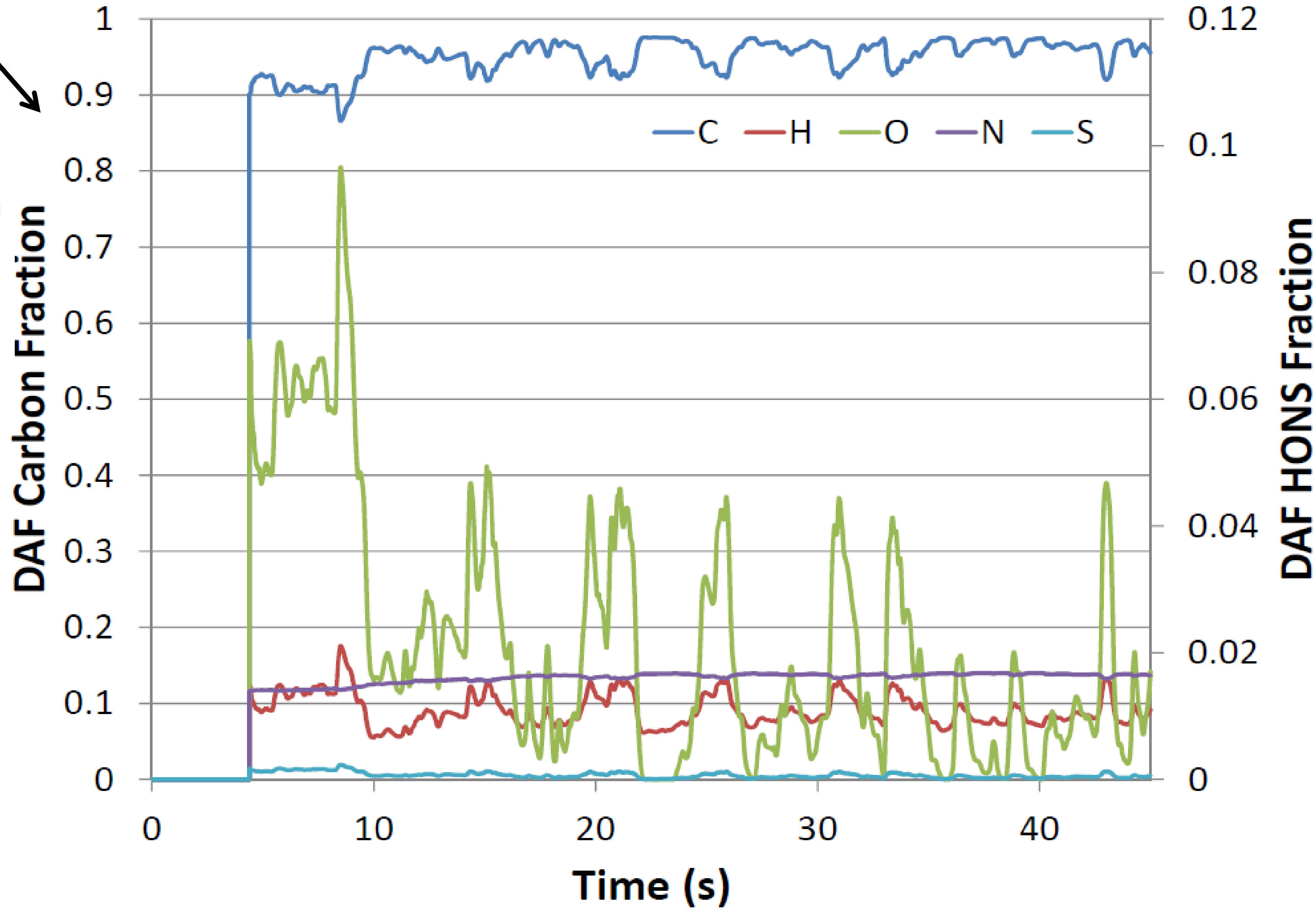
Example Test Case



Char Composition at Exit



The important takeaway is that this method allows char to be represented by more than just carbon and that the exit composition is relatively close to PCCL predictions

Where Can You Find C3M?

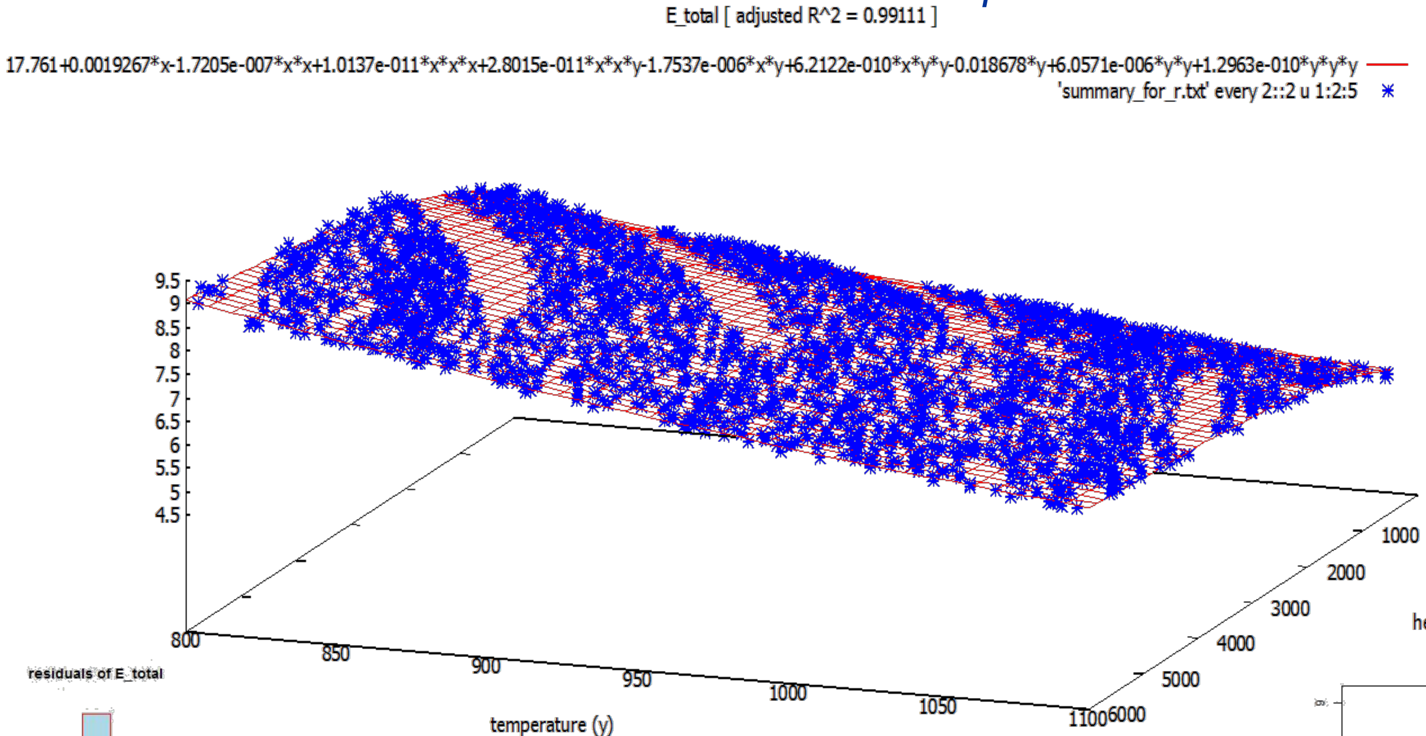
https://mfix.netl.doe.gov/members/download_C3M.php

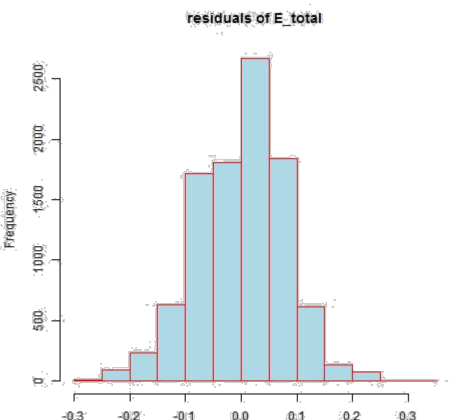
Thank You for Your Attention!

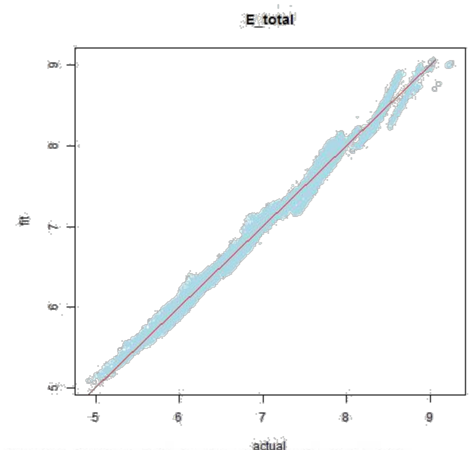
Reserve Slides

What’s New in C3M?

Surface Response Modeling with CHONS Coal
PCCL with PRB Example

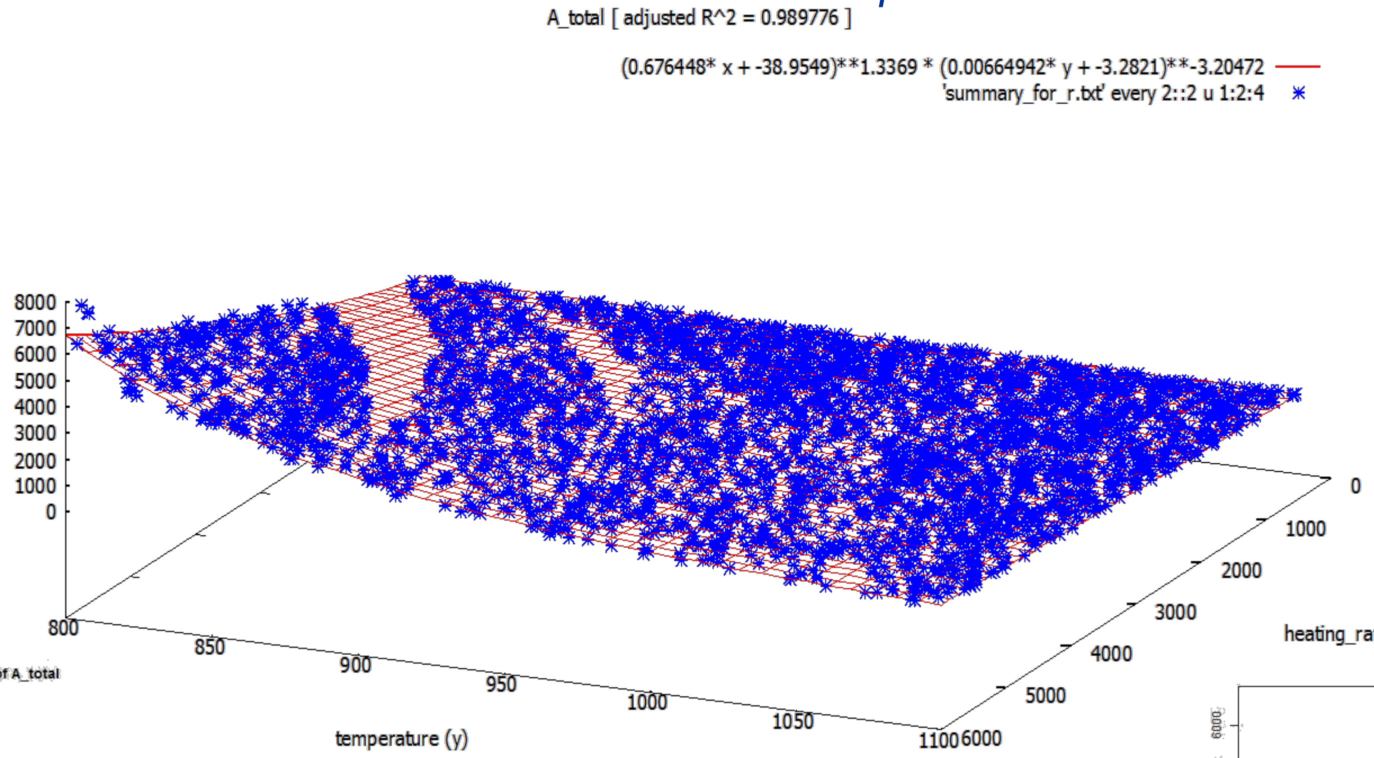


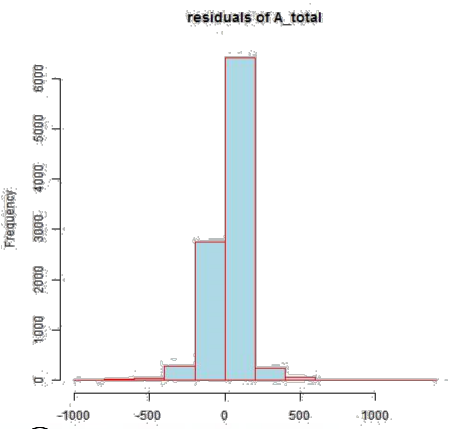


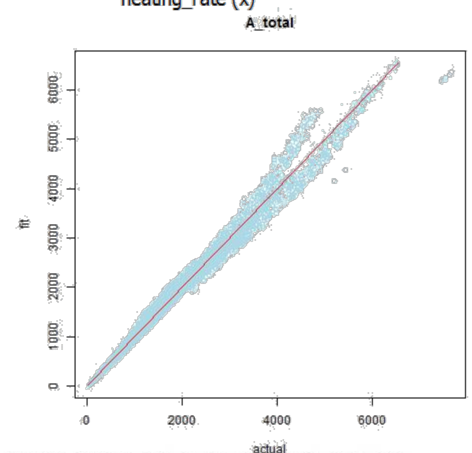


What’s New in C3M?

Surface Response Modeling with CHONS Coal
PCCL with PRB Example







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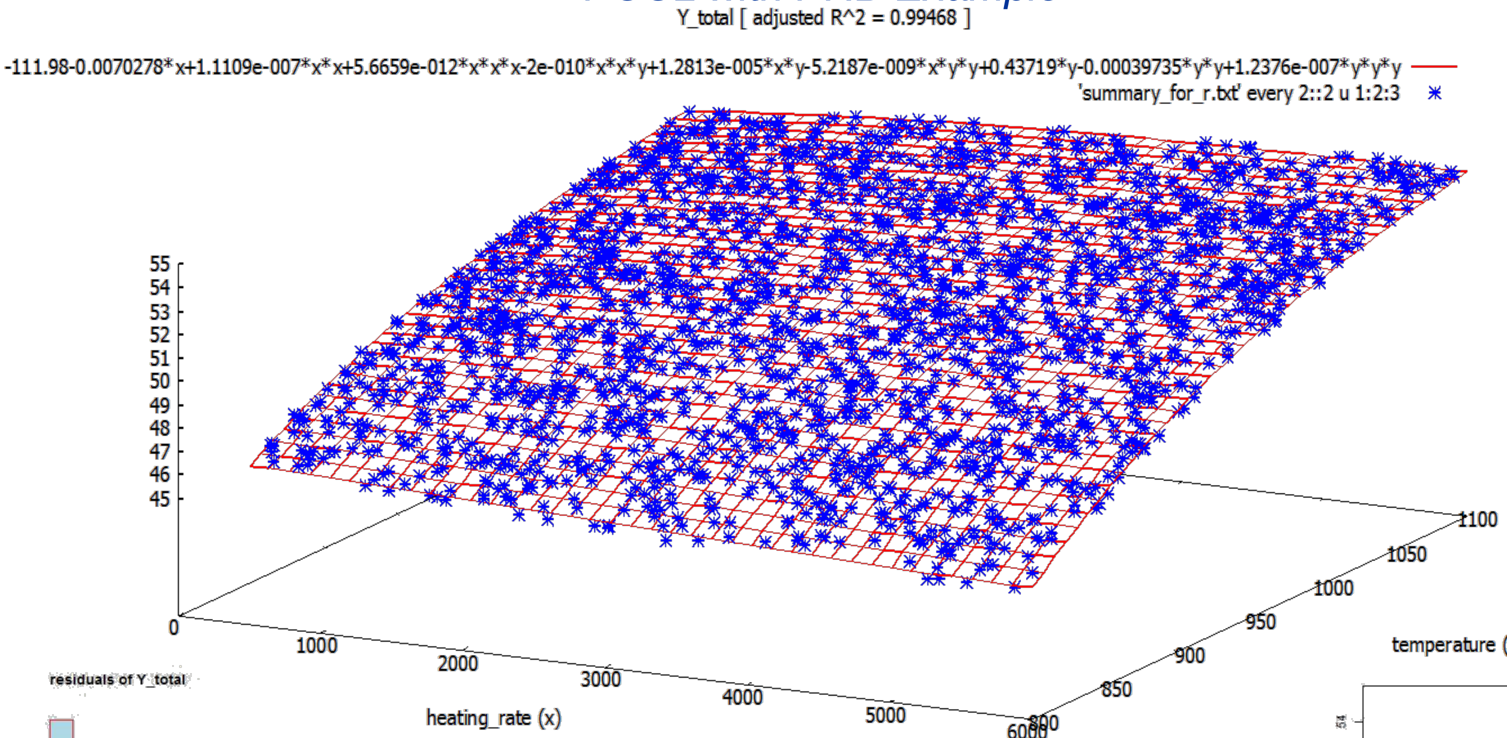
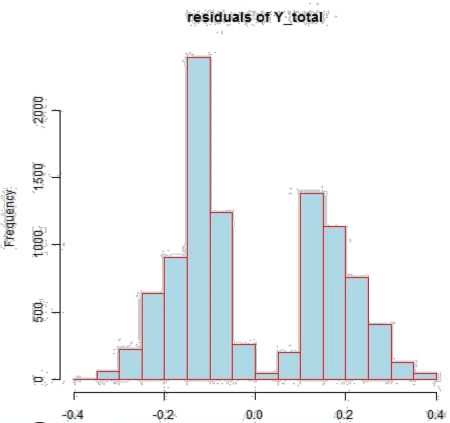
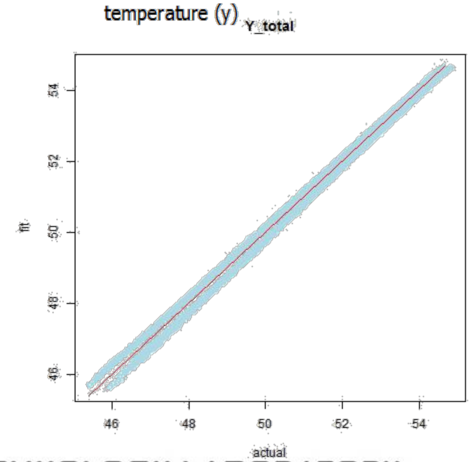
Surface Response Modeling with CHONS Coal
PCCL with PRB Example

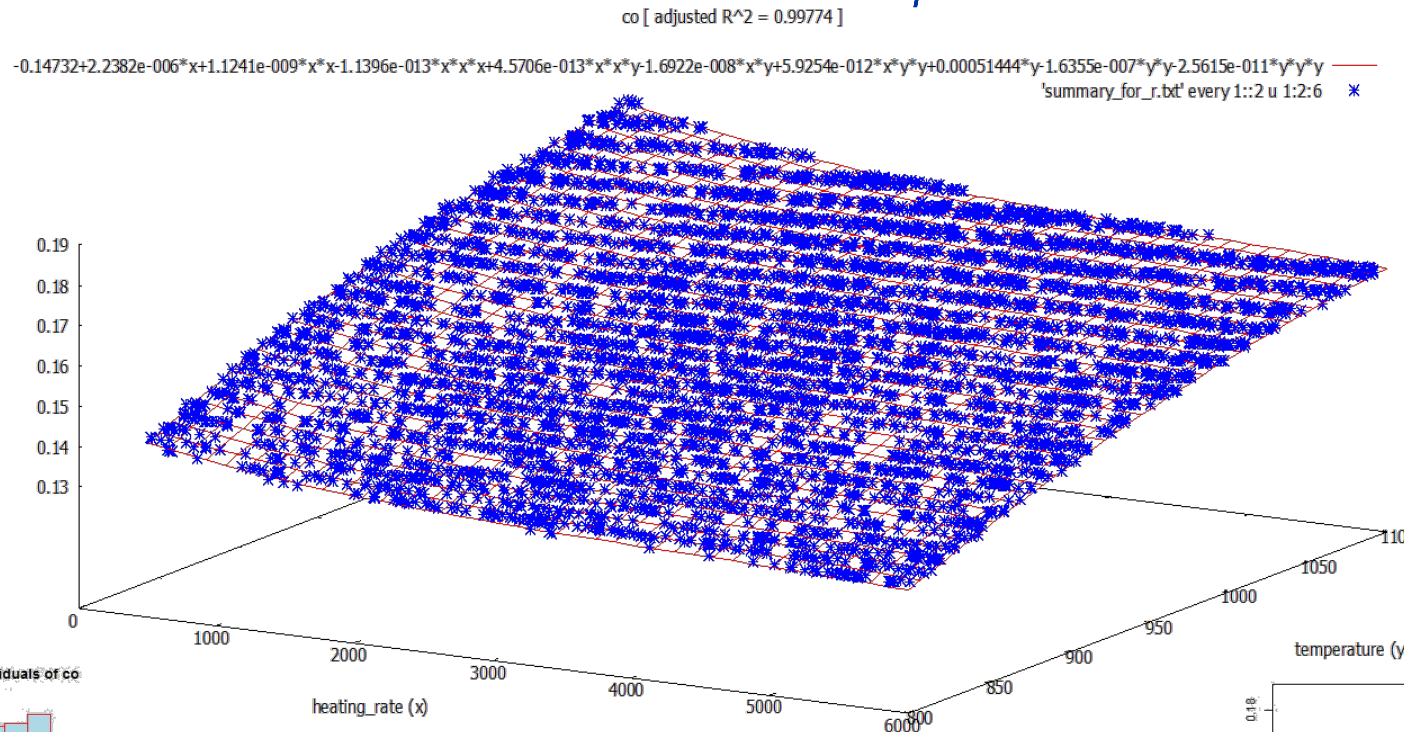


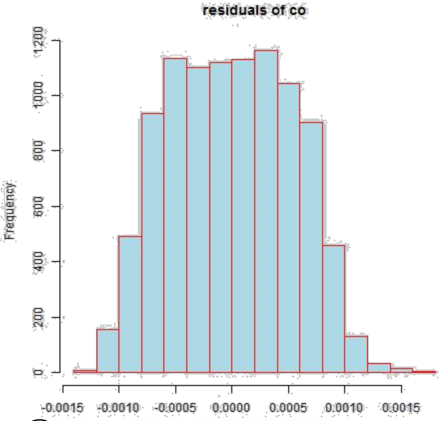


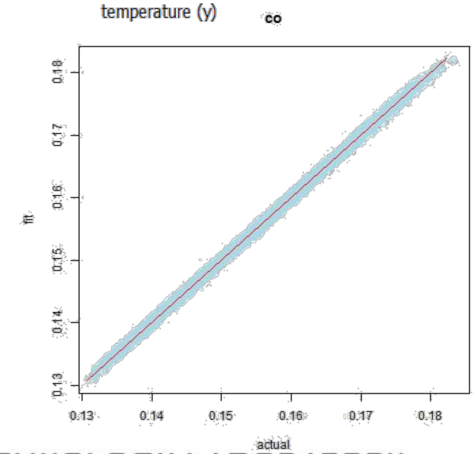


What’s New in C3M?

Surface Response Modeling with CHONS Coal
PCCL with PRB Example

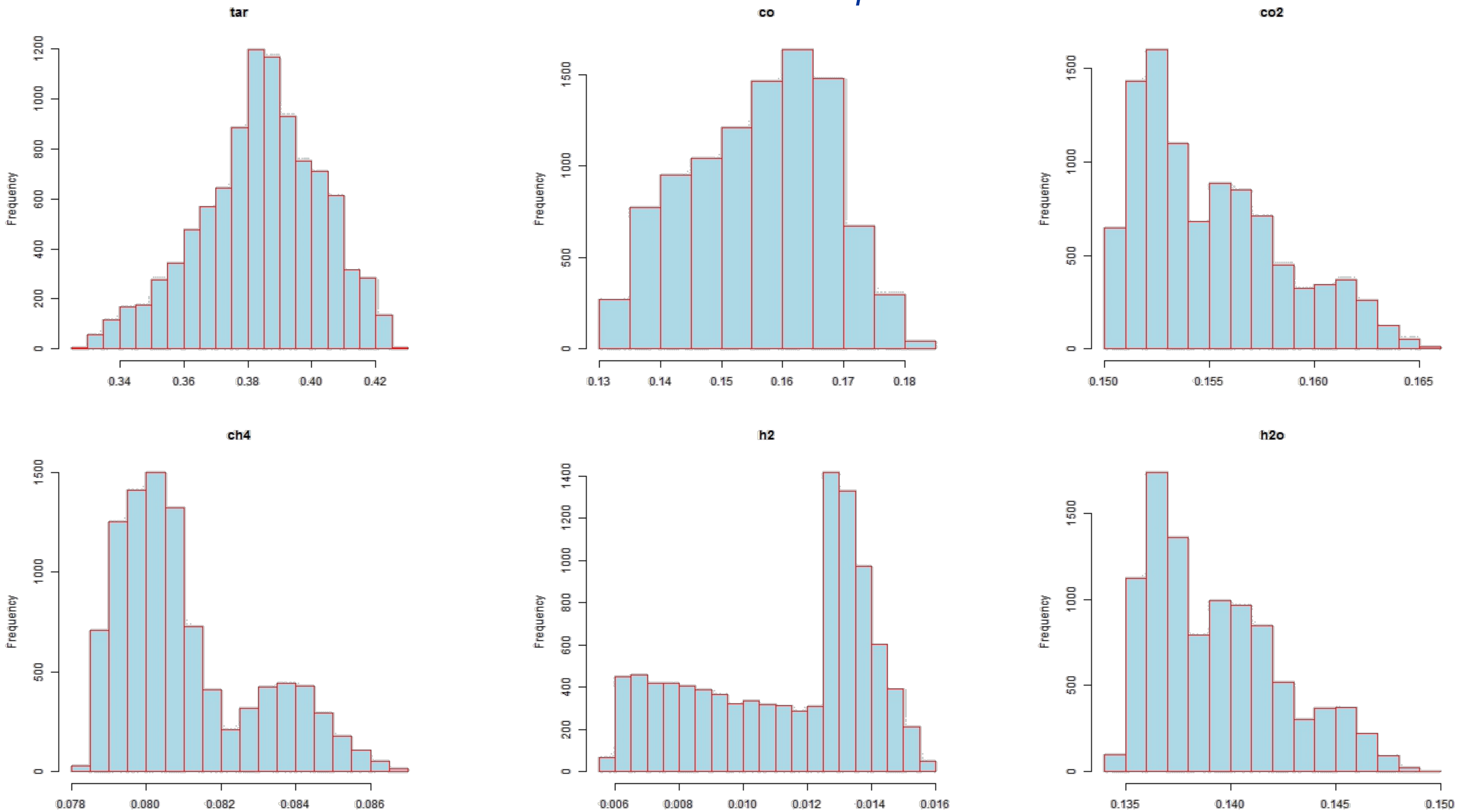






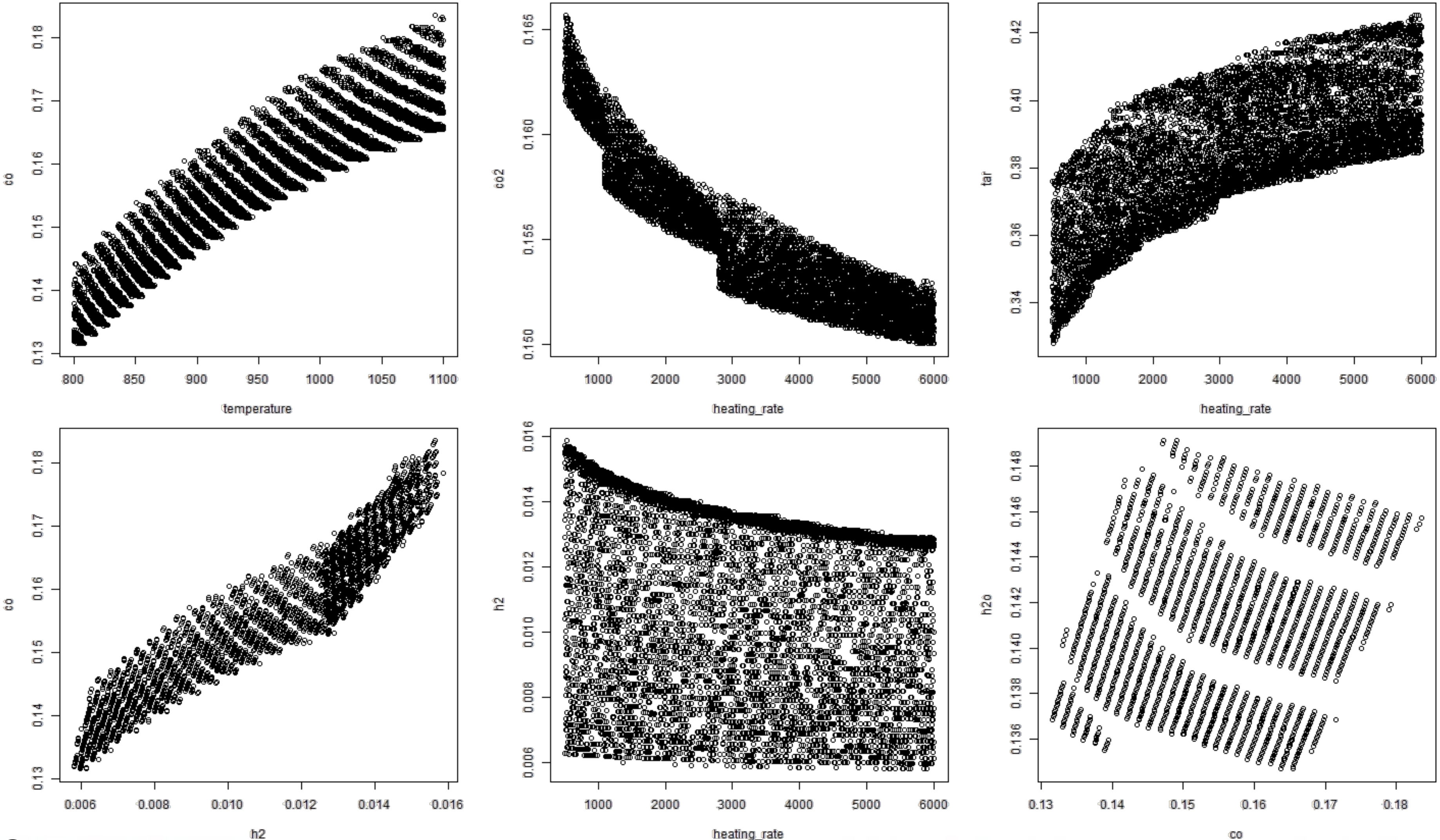
What's New in C3M?

Uncertainty Quantification
PCCL with PRB Example

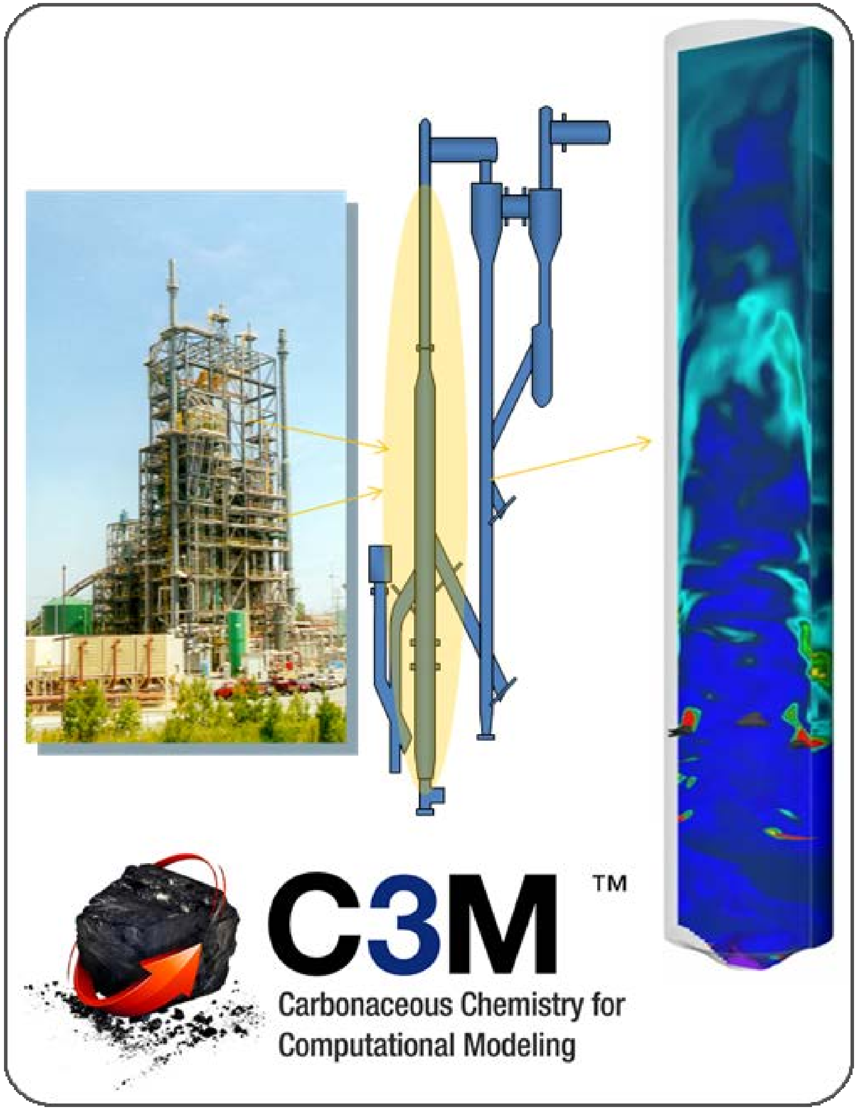


What's New in C3M?

Uncertainty Quantification
PCCL with PRB Example

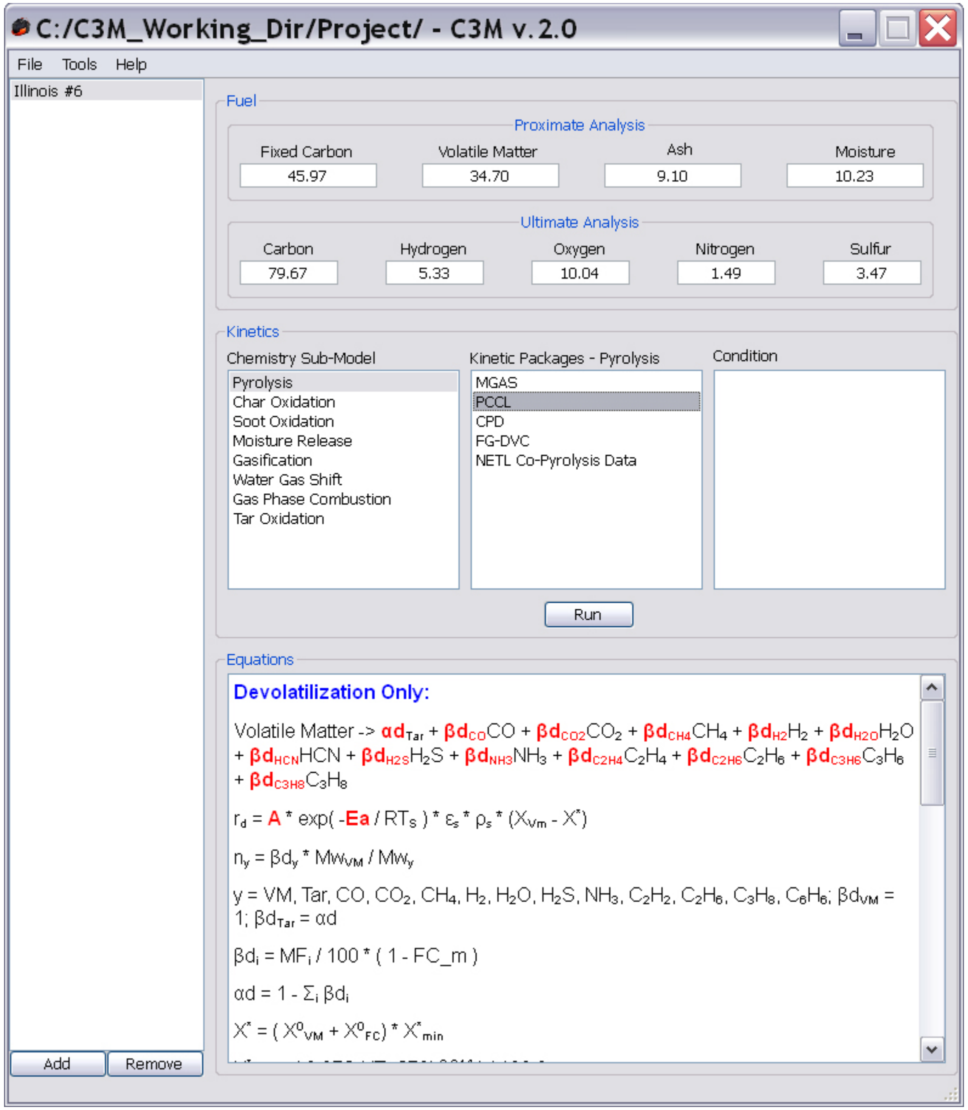


Work Flow: Open C3M

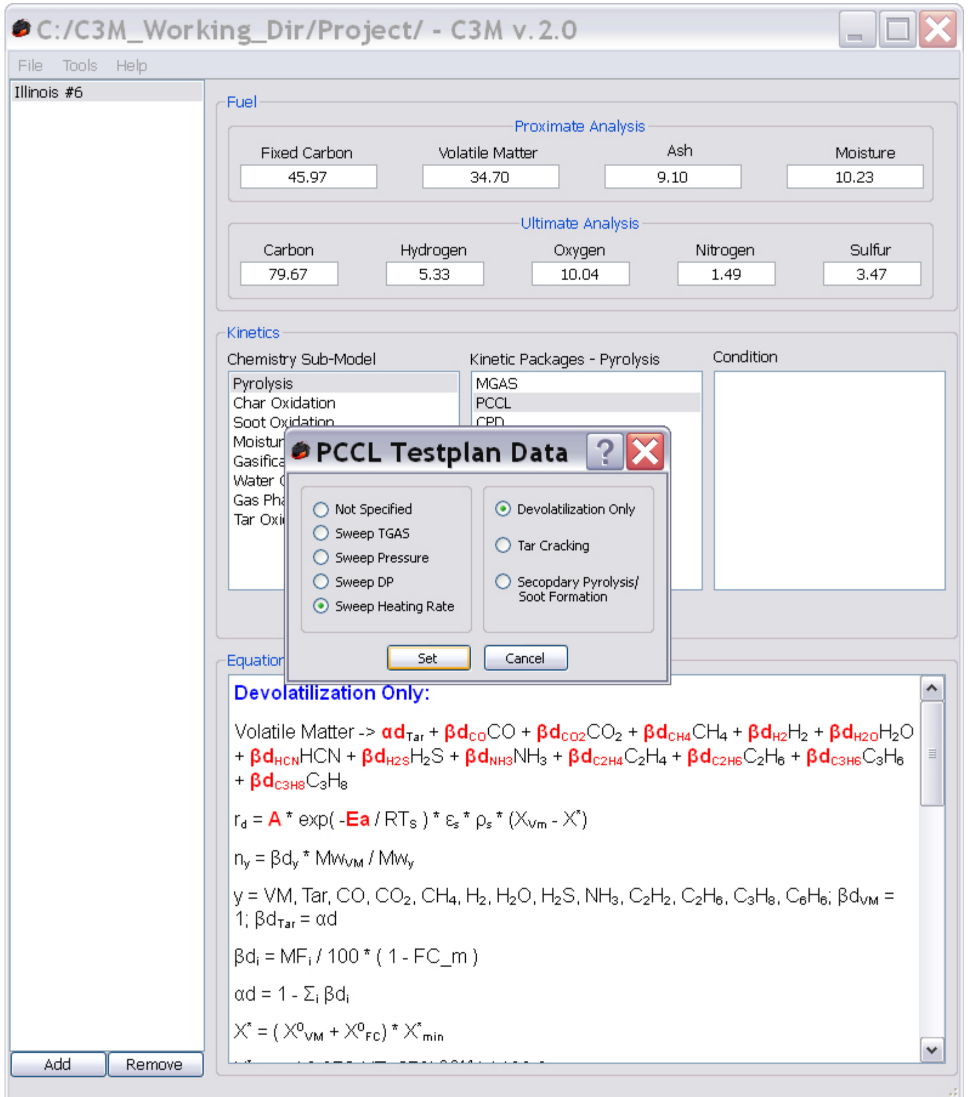


Work Flow: Input Standard Fuel Properties

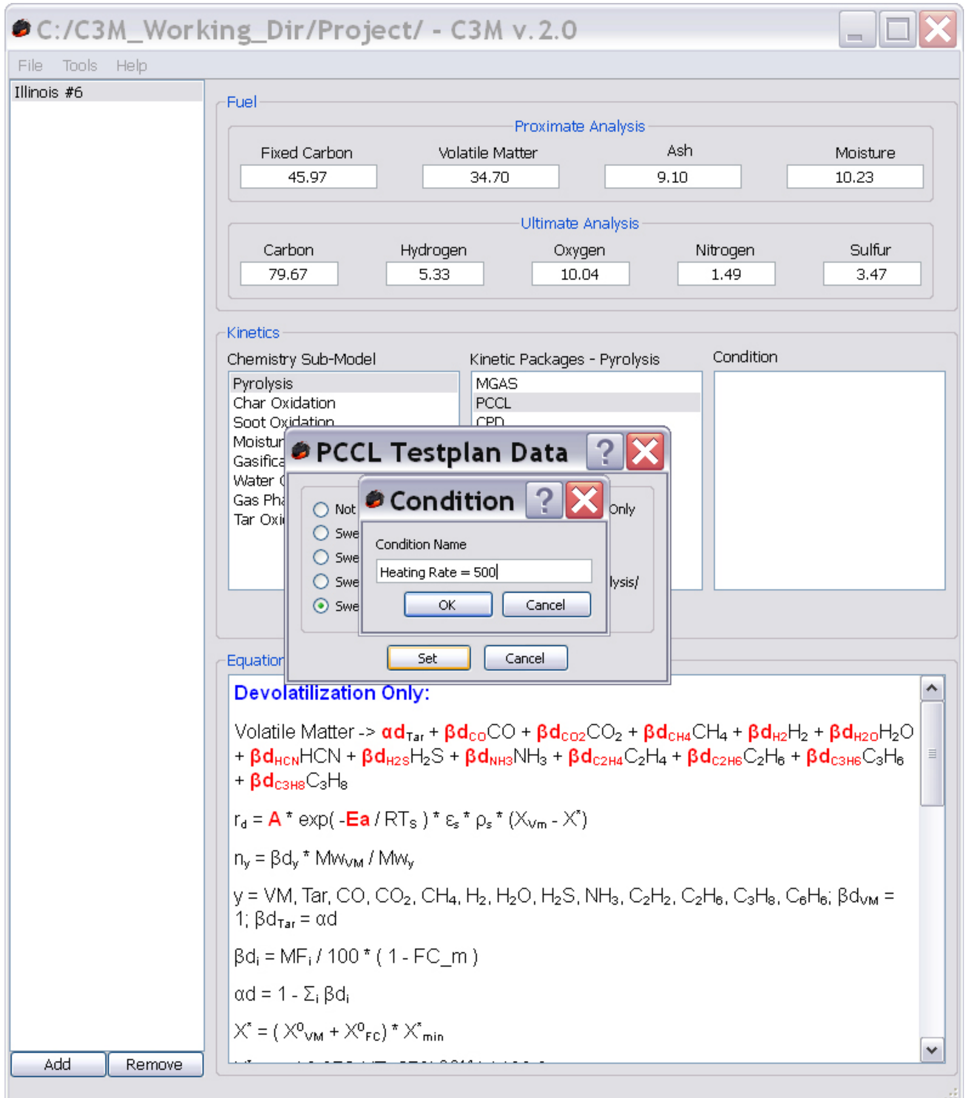
Work Flow: Run All Desired Sub-Models



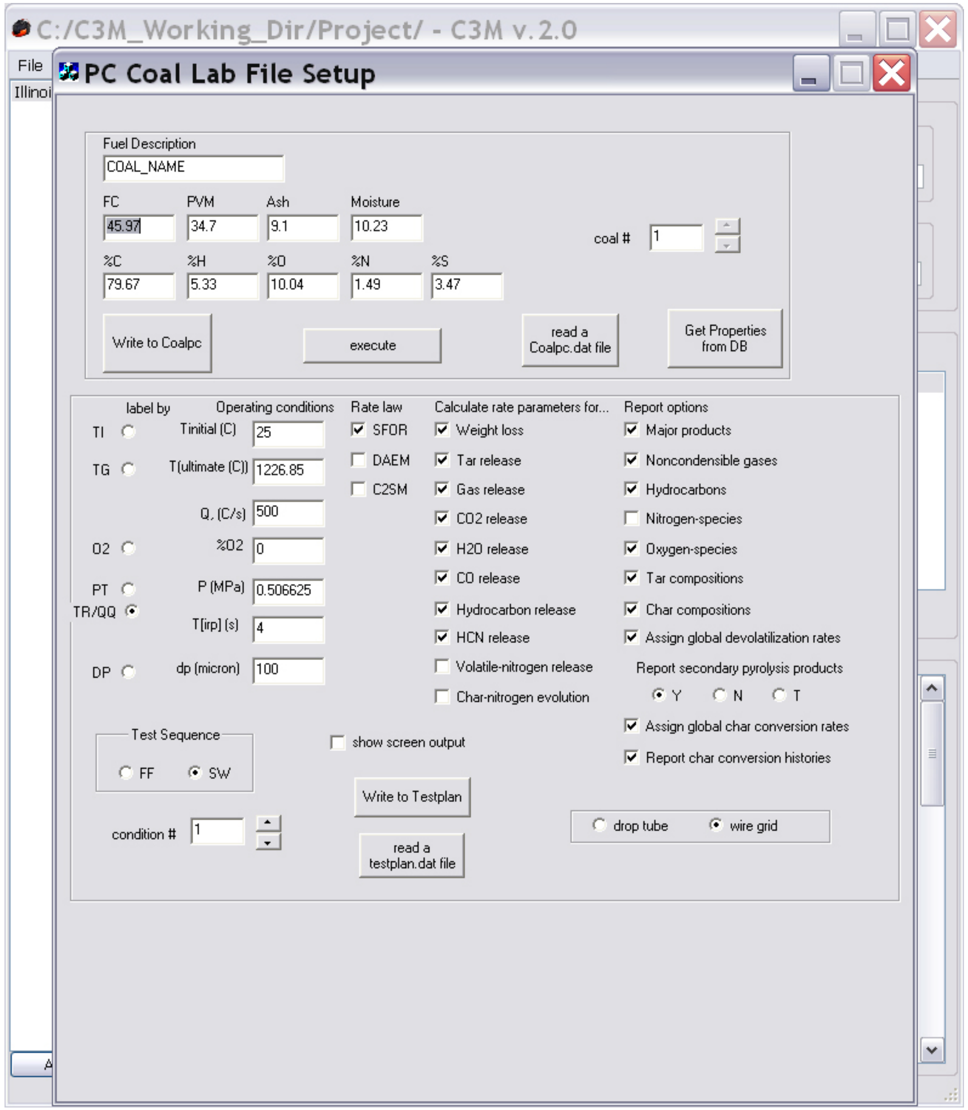
Work Flow: Run All Desired Sub-Models



Work Flow: Run All Desired Sub-Models



Work Flow: Run All Desired Sub-Models



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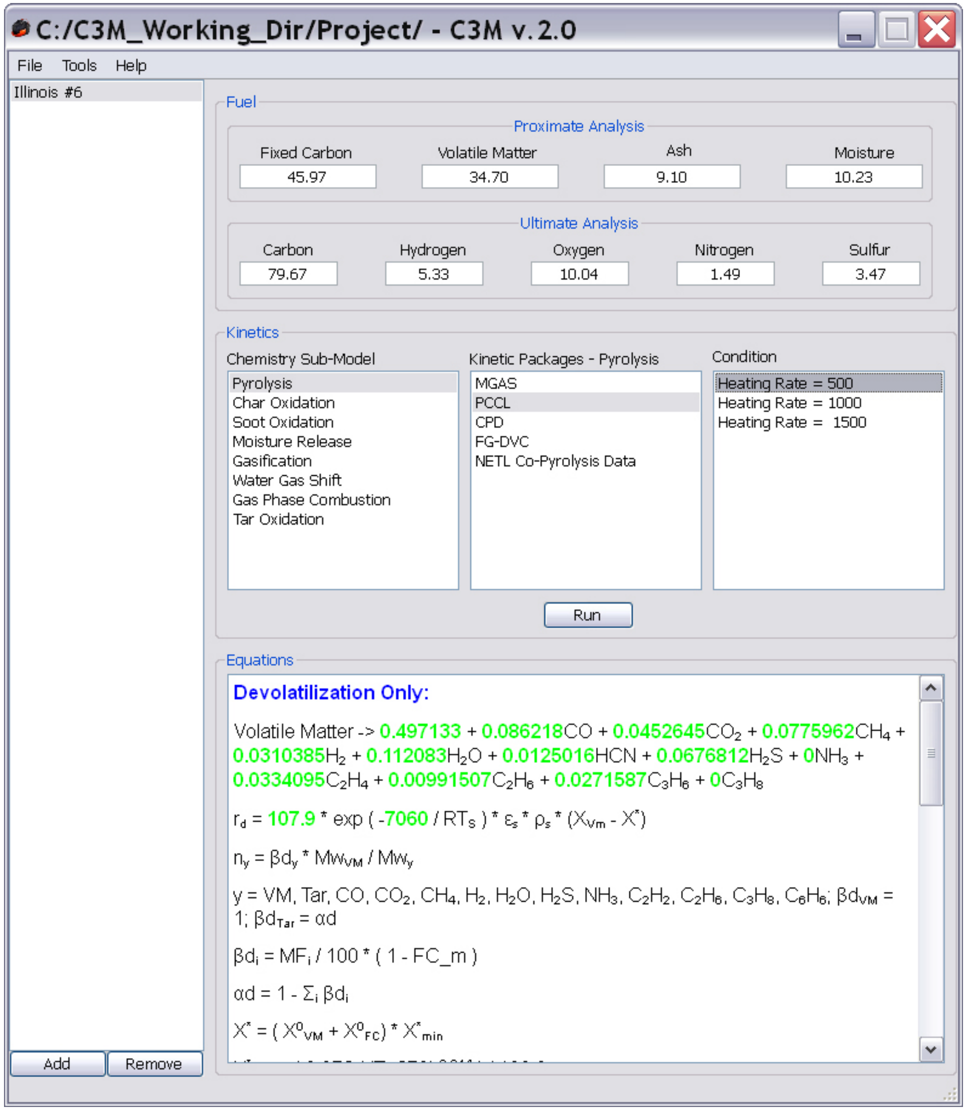
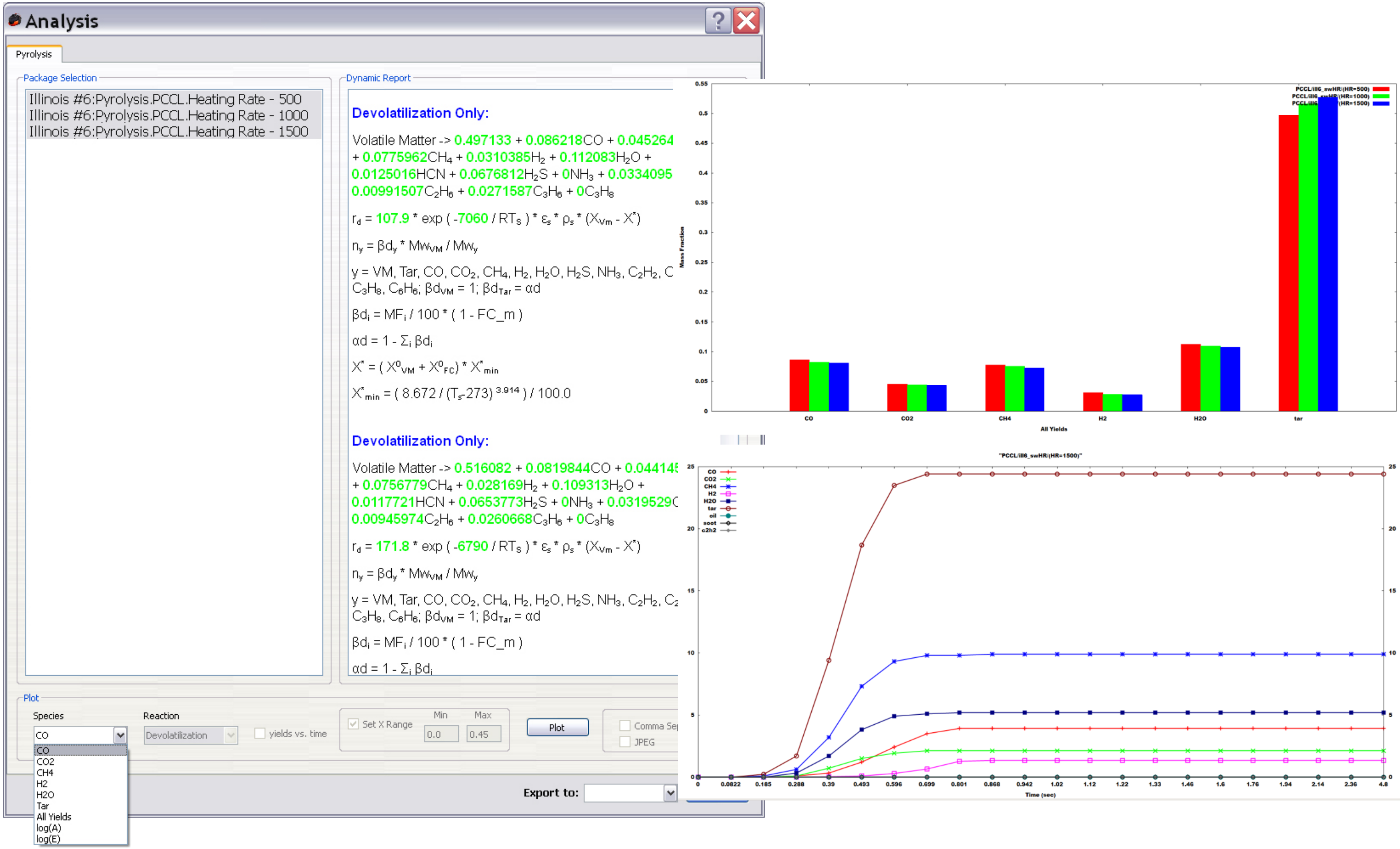
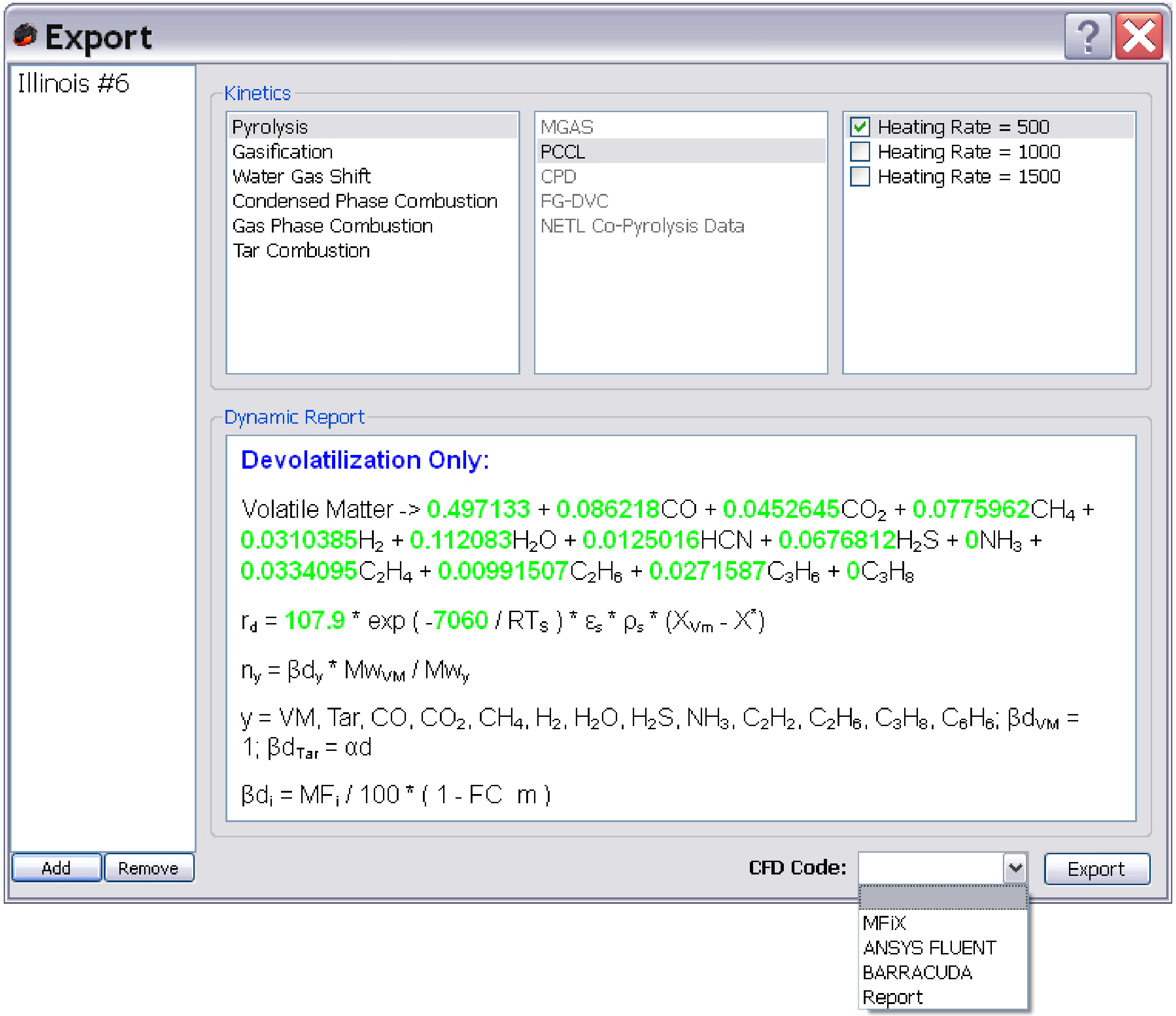


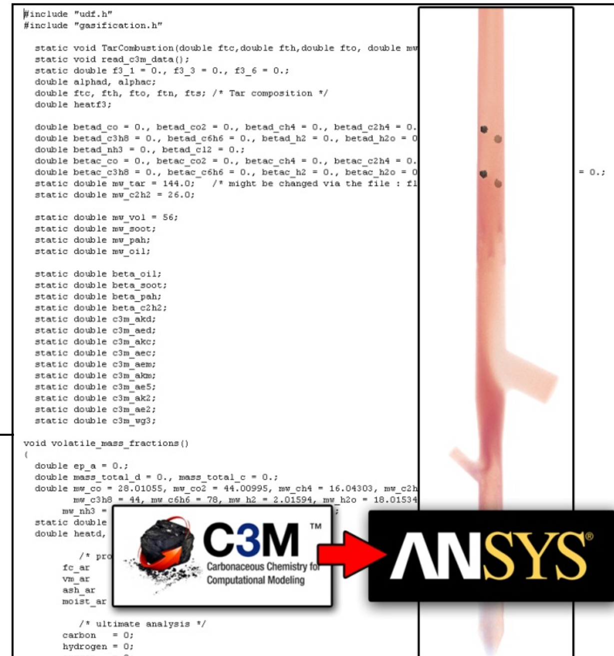
Work Flow: Compare Results

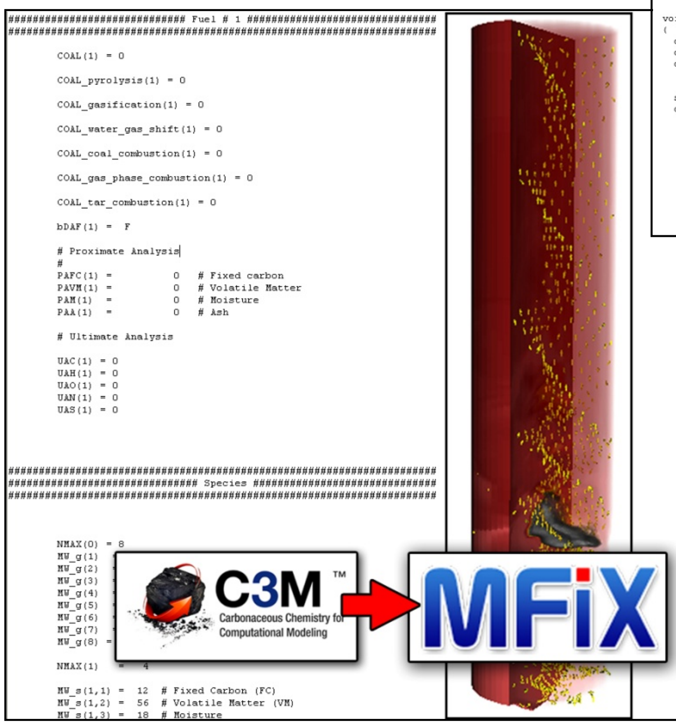


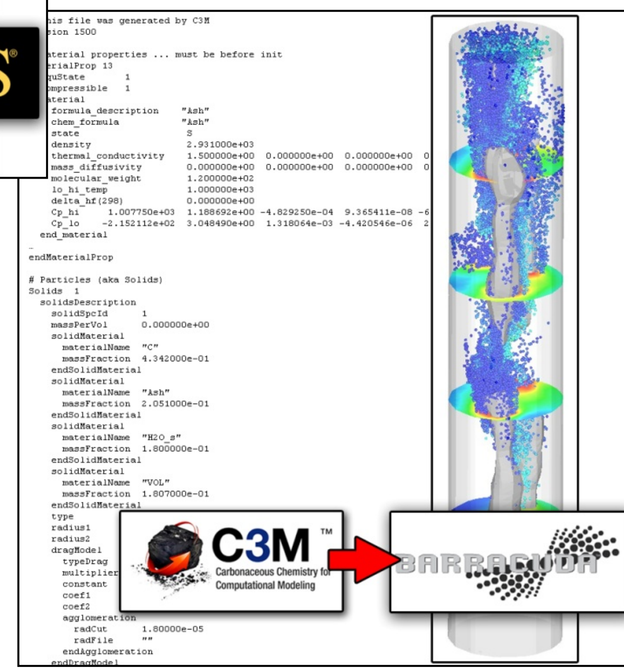
Work Flow: Select Input for Global Model



Work Flow: Generate Input Files for CFD







The Future of C3M

Uncertainty Quantification

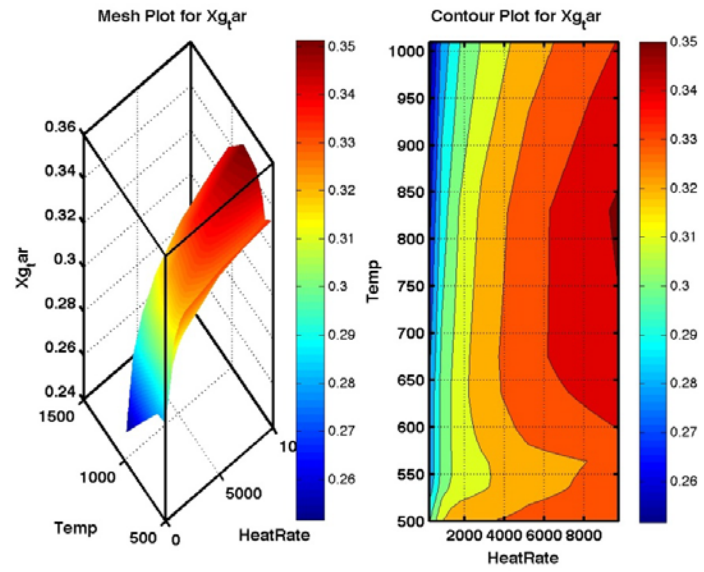
- **In order to accelerate technology deployment from pilot scale to commercial scale, CFD model predictions have to take into account and quantify various sources of uncertainty.**
  - Identify and characterize all sources of uncertainty (Aleatory or Epistemic)
  - uncertainty due to numerical approximations (discretization, round off, convergence)
  - Propagate input uncertainties through the model
  - Estimate model form uncertainty
  - Determine total uncertainty in the predicted system response
- **In order to assess uncertainty in CFD, one has to assess the uncertainty in kinetics, which means that C3M must be able to produce Probability Distribution Functions (PDF, not to be confused with portable document files) to pass to a CFD code**

The Future of C3M

Uncertainty Quantification

Example: Gas Production response to Heating Rate, Temp., and Press. within the PCCL pyrolysis model

- **Uncertain input parameters**
  - Heating rate (oC/s) [200 – 9727]
  - Temperature (oC) [500 – 1010]
  - Pressure (kPa) [861 – 3447]
- **Response surfaces for output variables such as volatile gases are generated**
- **PSUADE UQ toolbox is used to generate PDFs for input parameters for Monte Carlo simulations:**
  - Heating rate: Normal (μ = 3000, σ = 1000)
  - Temperature: Normal (μ = 800, σ = 100)
  - Pressure: Normal (μ = 2000, σ = 500)
- **Propagation of input uncertainties are examined by 10,000 Direct MC simulation and 10,000 MC simulation via surrogate model**

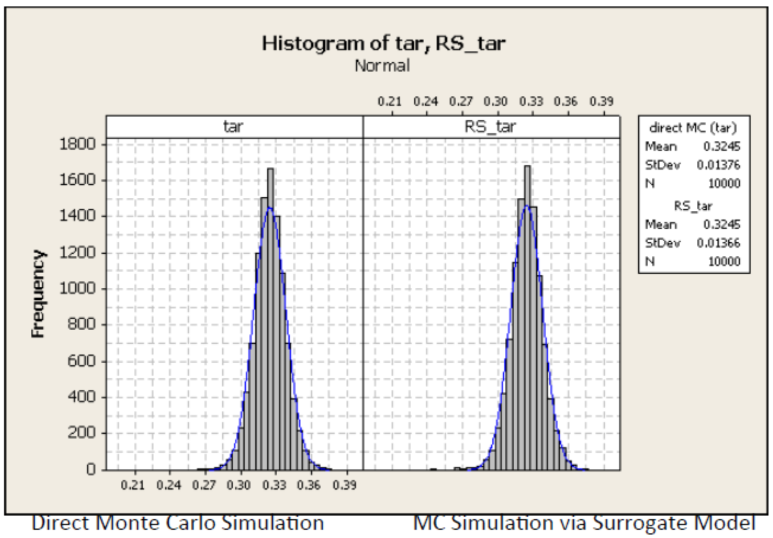


Response surface for propagating input uncertainty in tar pyrolysis process

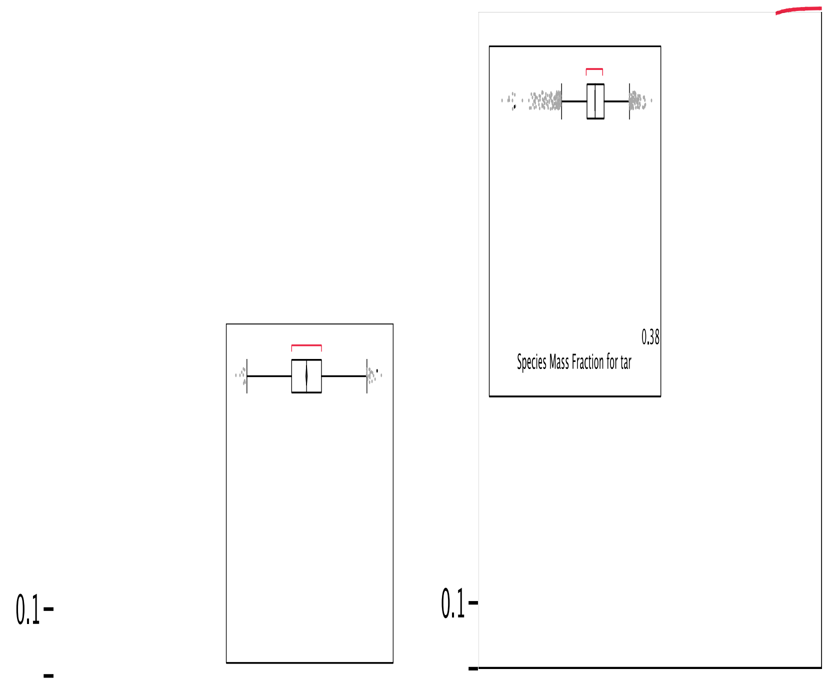
The Future of C3M

Uncertainty Quantification

Example: Gas Production response to Heating Rate, Temp., and Press. within the PCCL pyrolysis model



No major differences in the output parameters between direct MC simulation and MC simulation via surrogate model



Cumulative Density Function plots generated via Direct Monte Carlo simulation to assess the likelihood of achieving desired level of species under prescribed input uncertainties

The Future of C3M

Uncertainty Quantification

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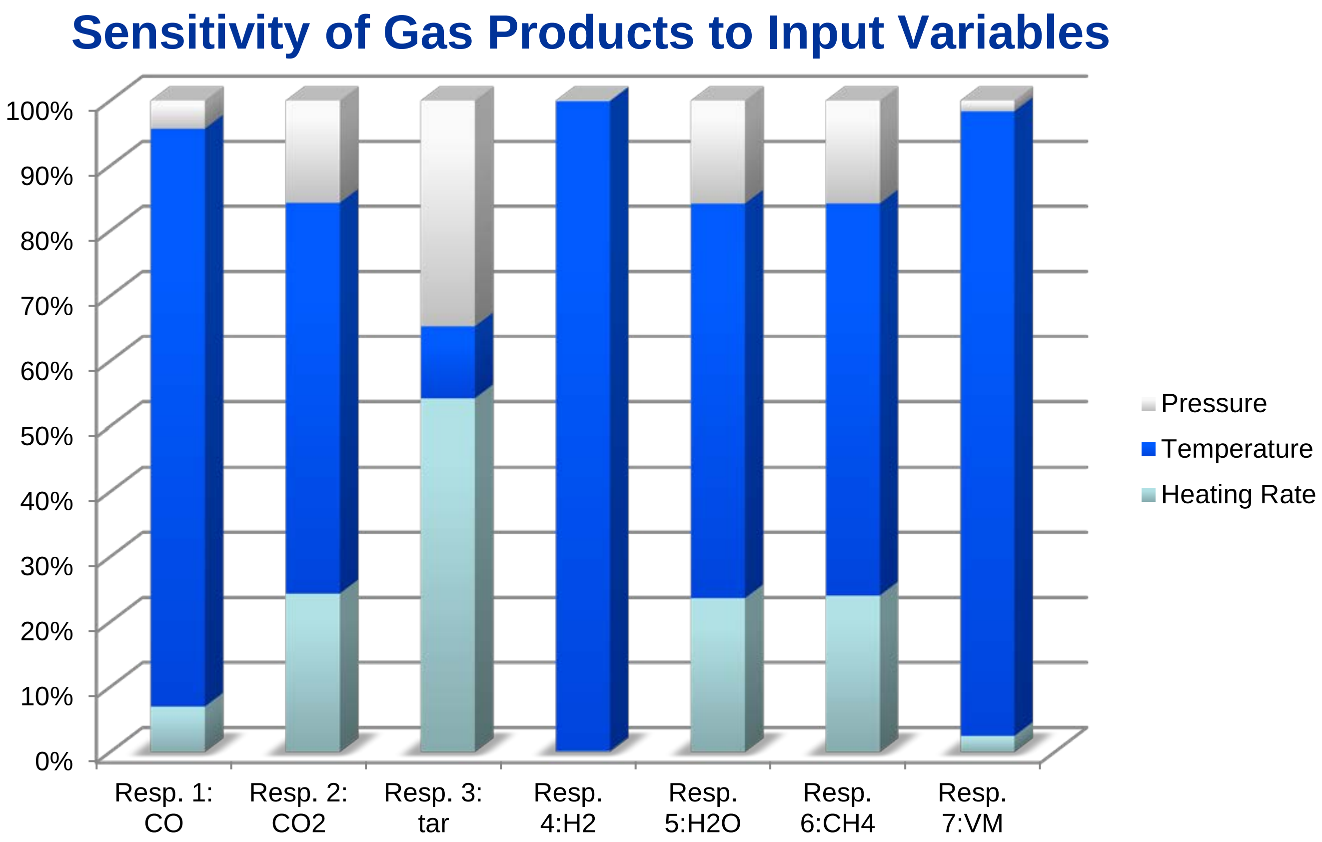


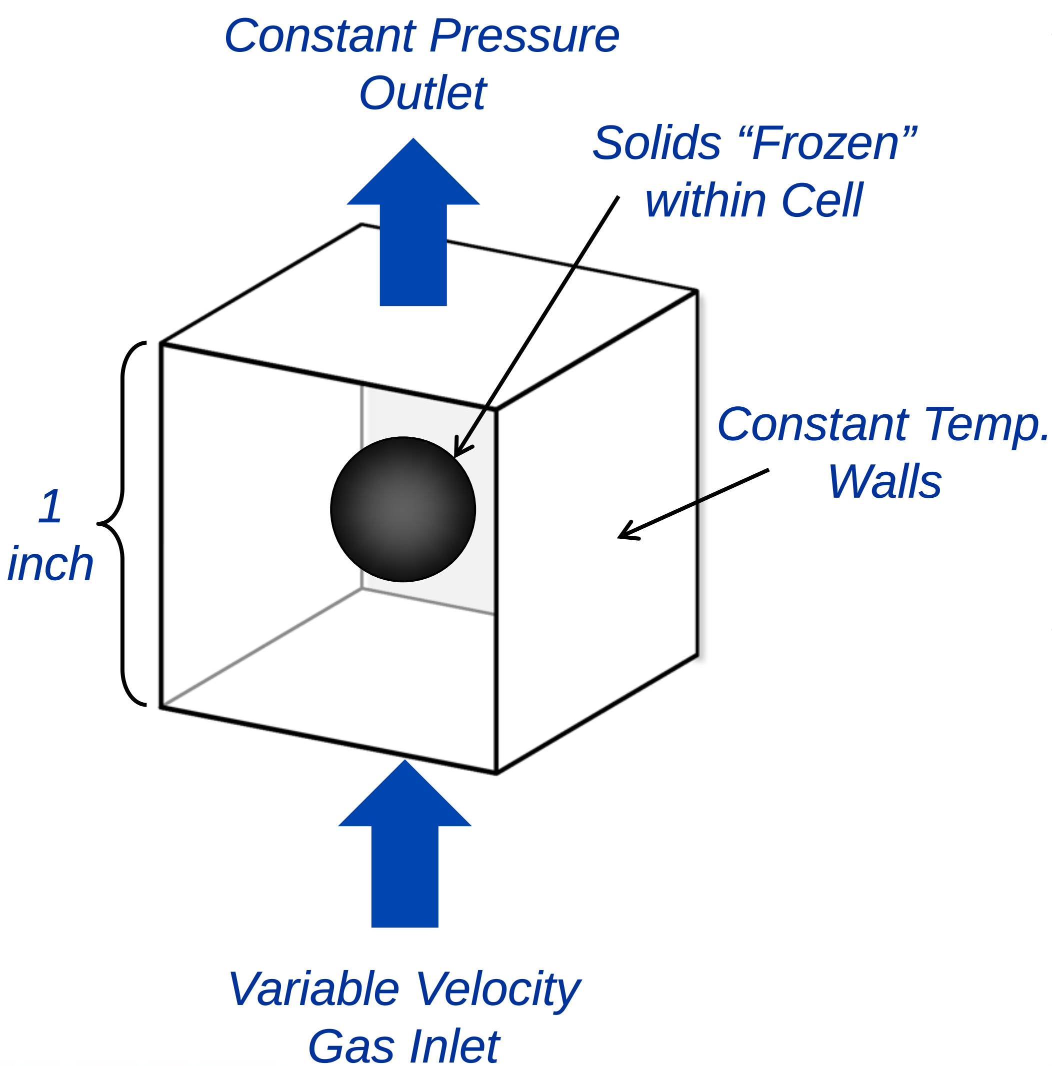
The Future of C3M

Uncertainty Quantification

- **The example was done manually with a lot of hard work**
- **Everything could be done programmatically**
- **Work plans call for development of a module within C3M that will allow for generation of response surfaces and PDF’s from any portion of the kinetics in C3M for any input variable.**

Work Flow: Run CFD with C3M Chemistry

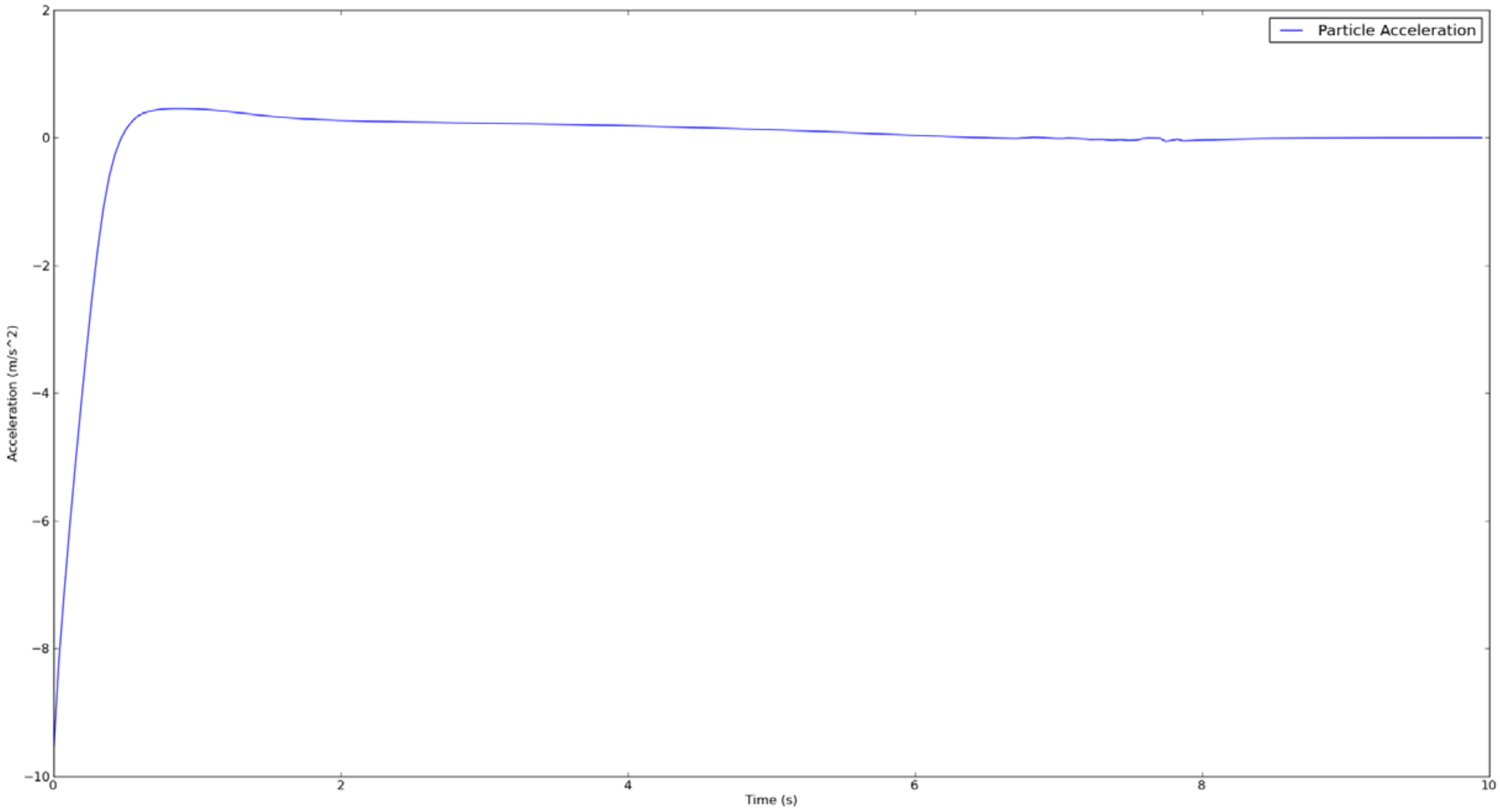
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



- **Initial Conditions**
  - V_{inlet_init} = 0.01 m/s
  - T_{gas_init} = 1200 K
  - T_{solid} = 300 K
  - D_p = 200 x10^{-6} m
  - θ_s = 0.001
  - ρ_s = Mixture Law
  - C_{s_init} = Set By C3M
  - C_{g_init} = [CO=.05, CO_2=.05, H_2=.05, O_2=0.1, H_2O=0.75]
- **Boundary Conditions**
  - P_{outlet} = 1 atm
  - T_{wall} = 1200 K
  - T_{gas_inlet} = 1200 K
  - V_{gas_inlet} = -SFFV
  - C_{g_inlet} = C_{g_init}

Work Flow: Analyze Results

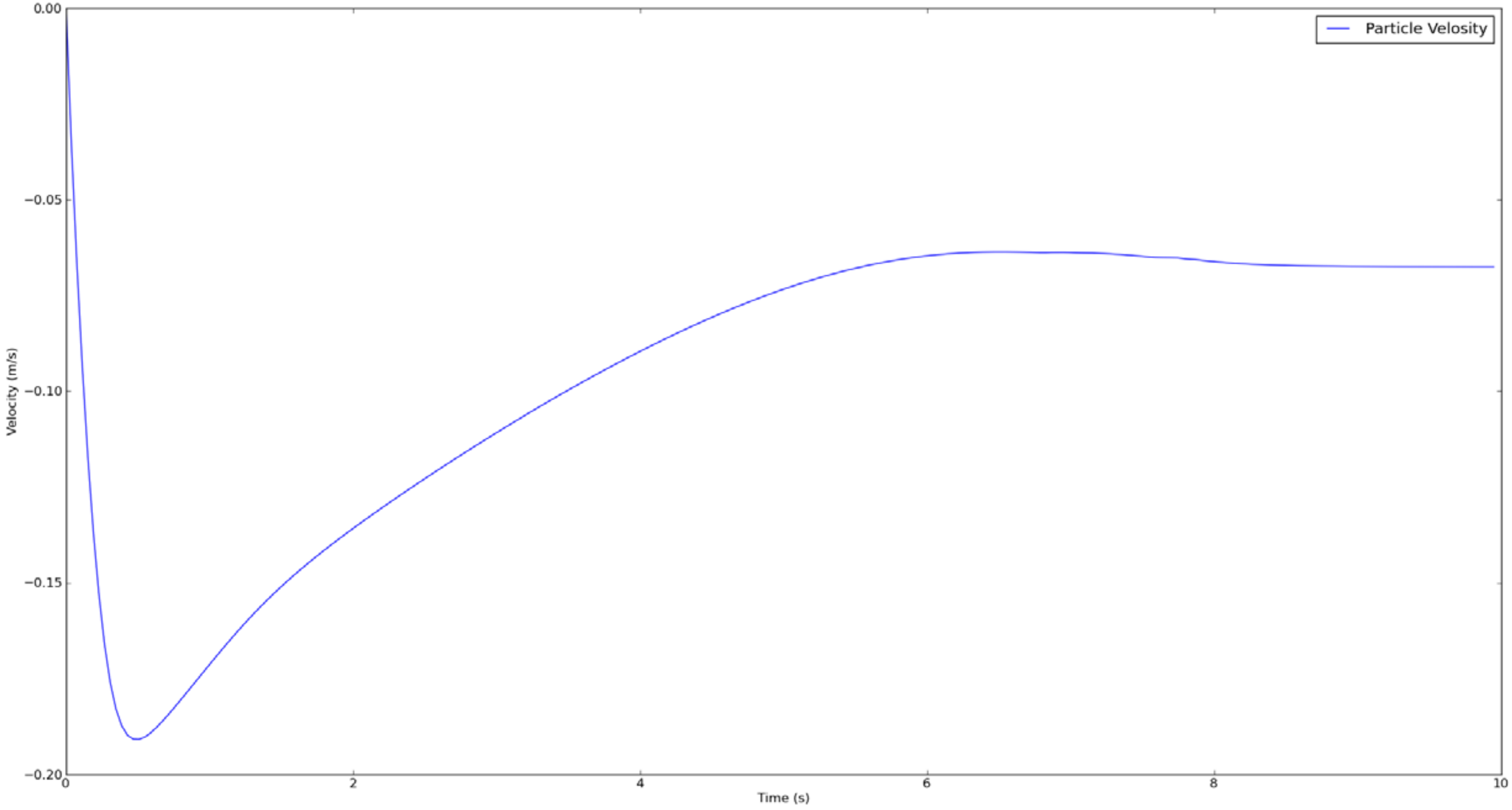
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



Result: Particle Acceleration

Work Flow: Setup and Run CFD

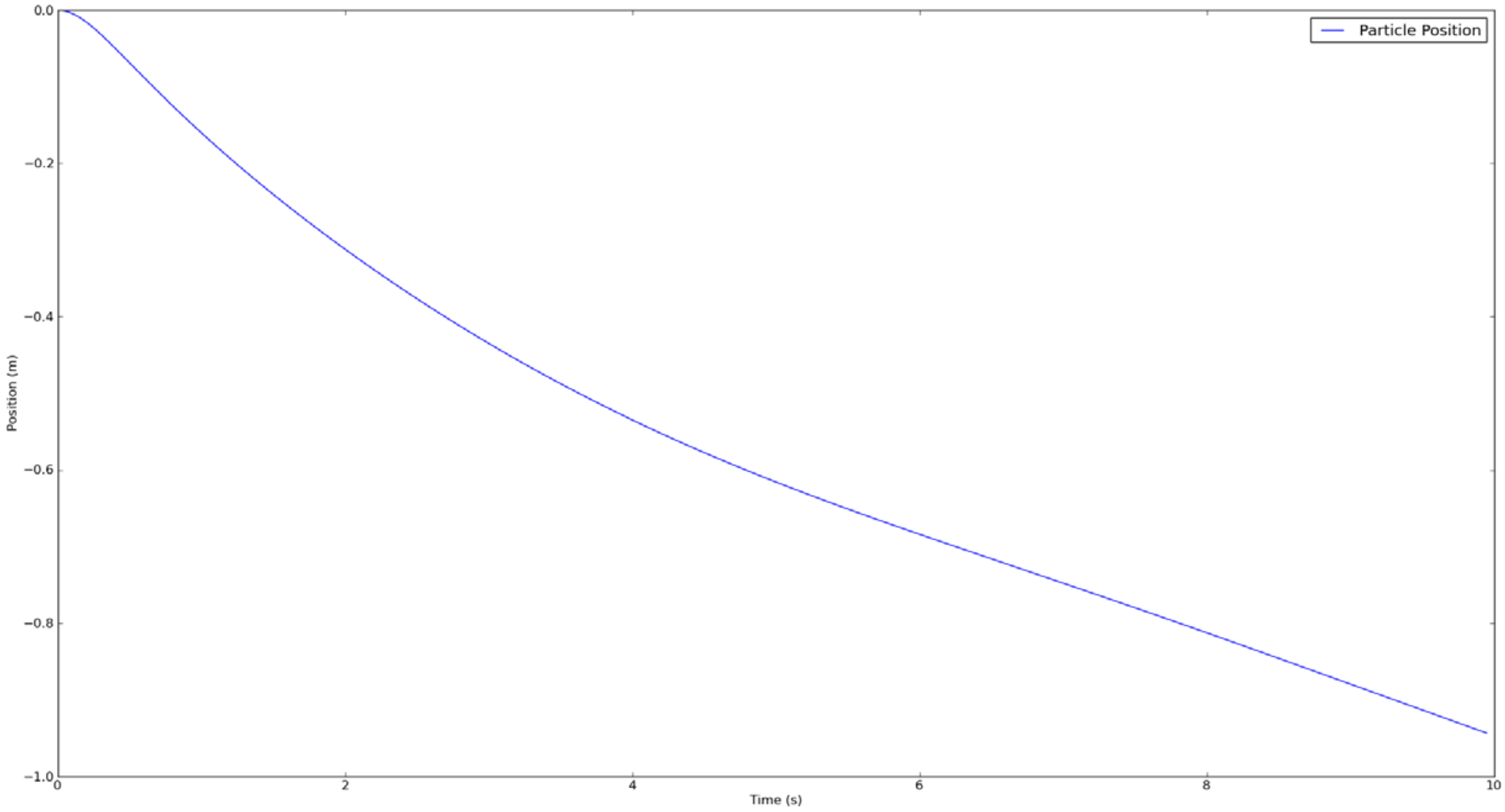
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



Result: Particle Velocity

Work Flow: Virtual Drop Tube

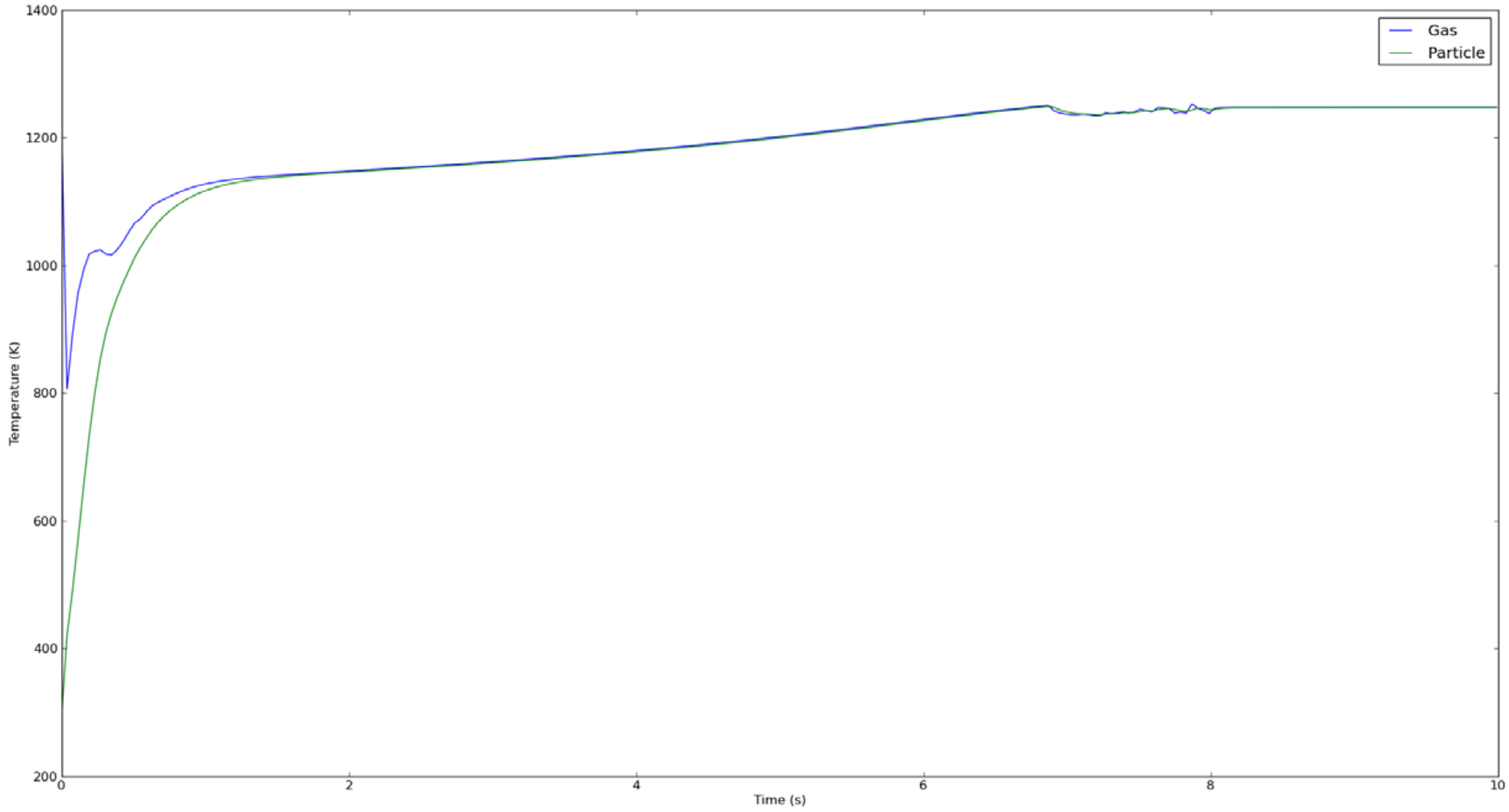
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



Result: Particle Position

Work Flow: Setup and Run CFD

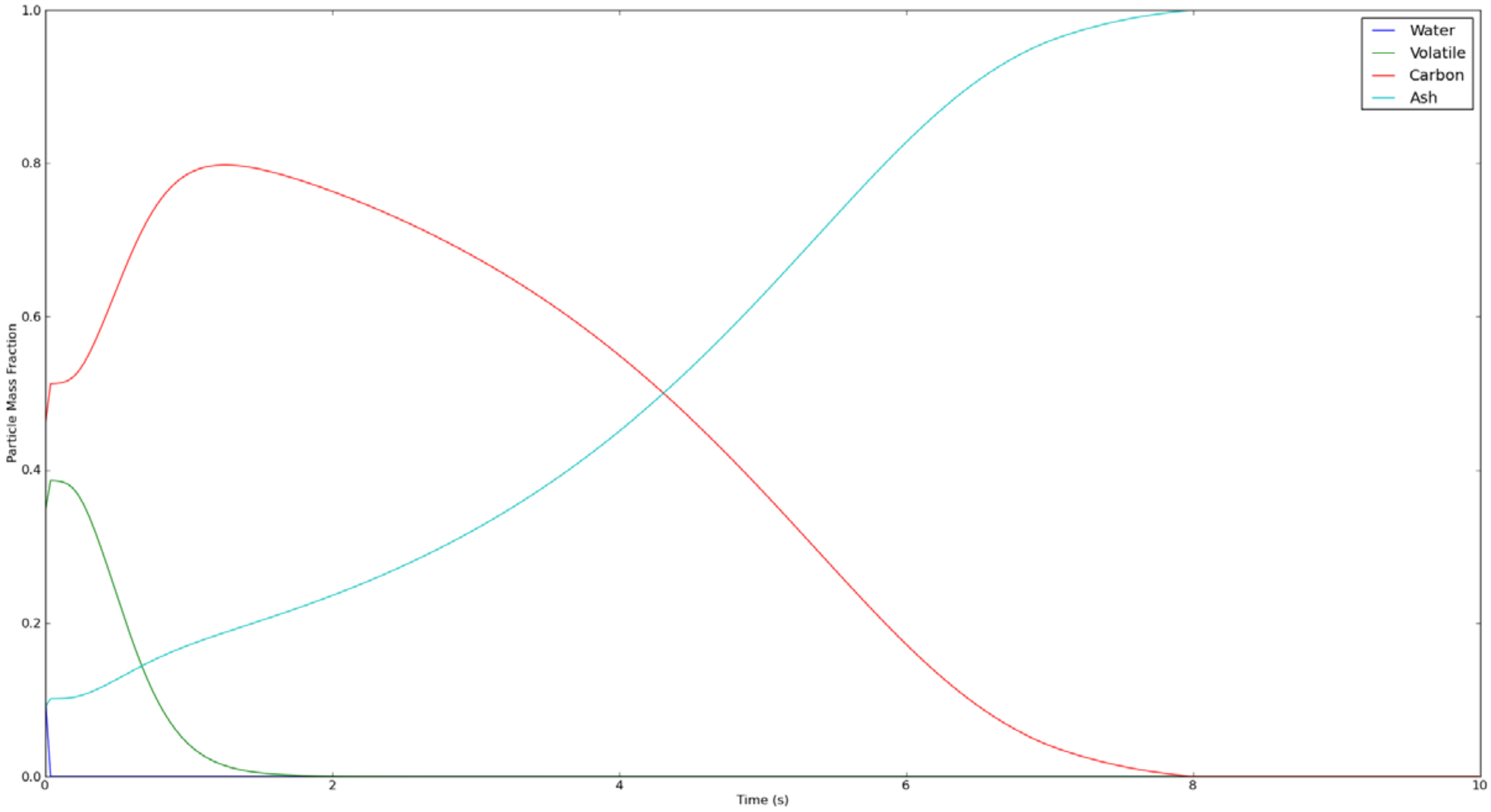
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



Result: Gas and Particle Temperature

Work Flow: Setup and Run CFD

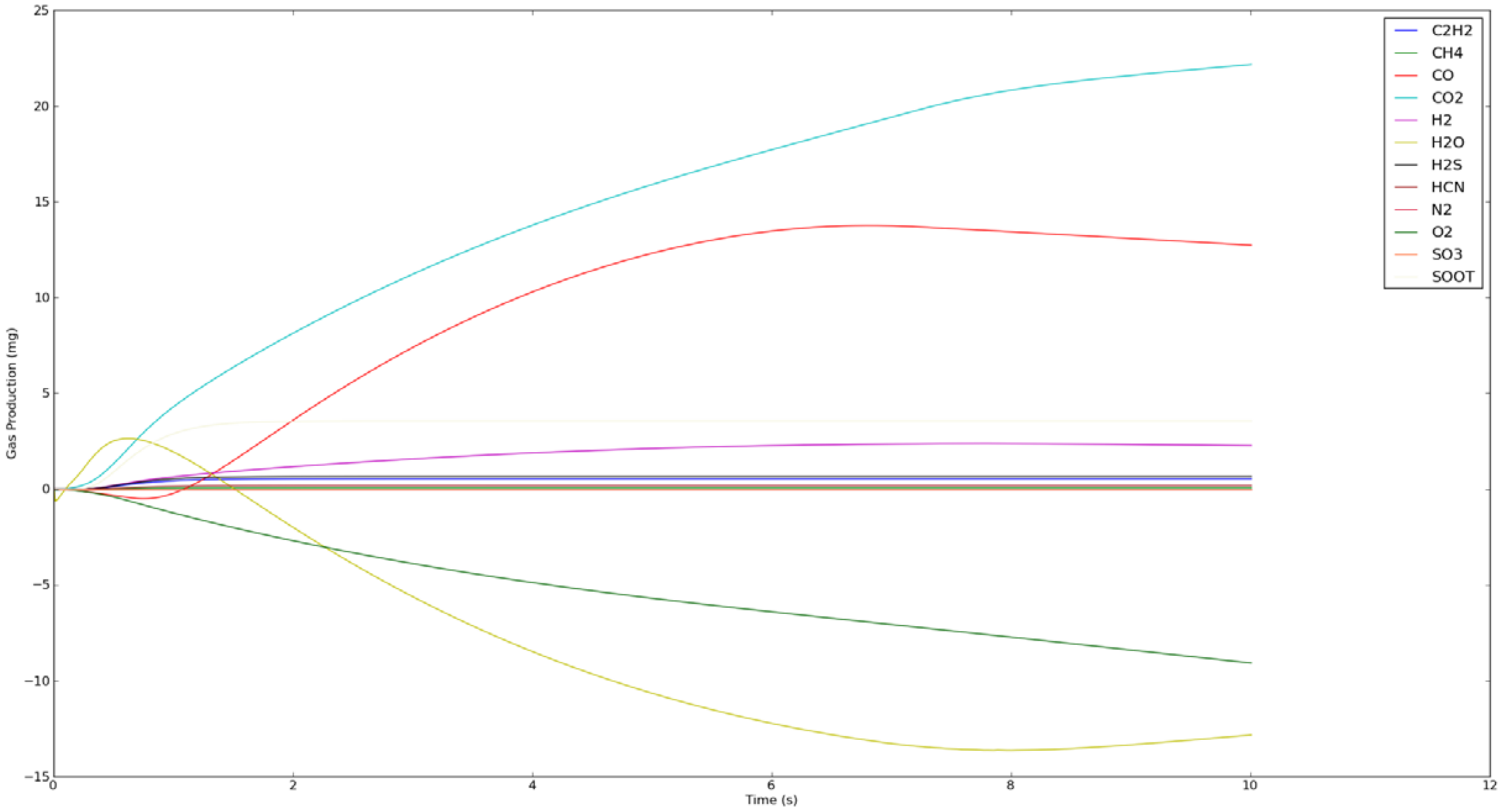
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



Result: Mass Fraction of Solid Species within Particle

Work Flow: Setup and Run CFD

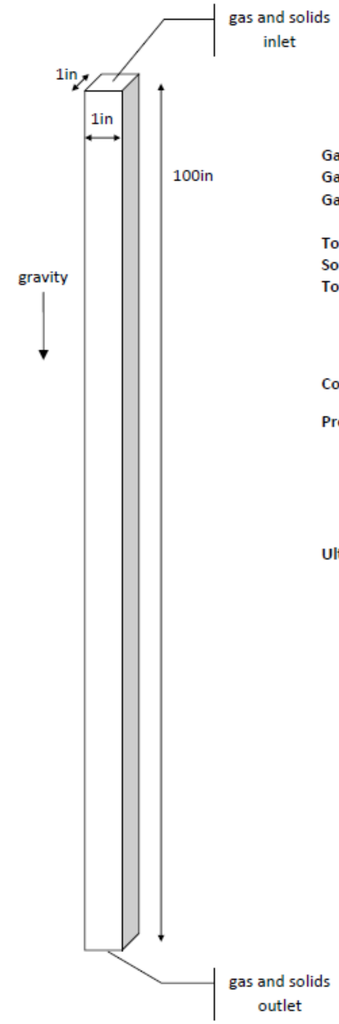
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



Result: Integration of Gas Species Flux Into and Out of System

Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



Gas velocity:	100 (cm/sec)
Gas Pressure:	1 (atm)
Gas Temperature:	1473.15 (K)
Total solids sample:	0.99866 (g)
Solids Feed Rate:	10,000 particles/sec
Total particles:	1,000

Coal Type: Rosebud

Proximate Analysis:

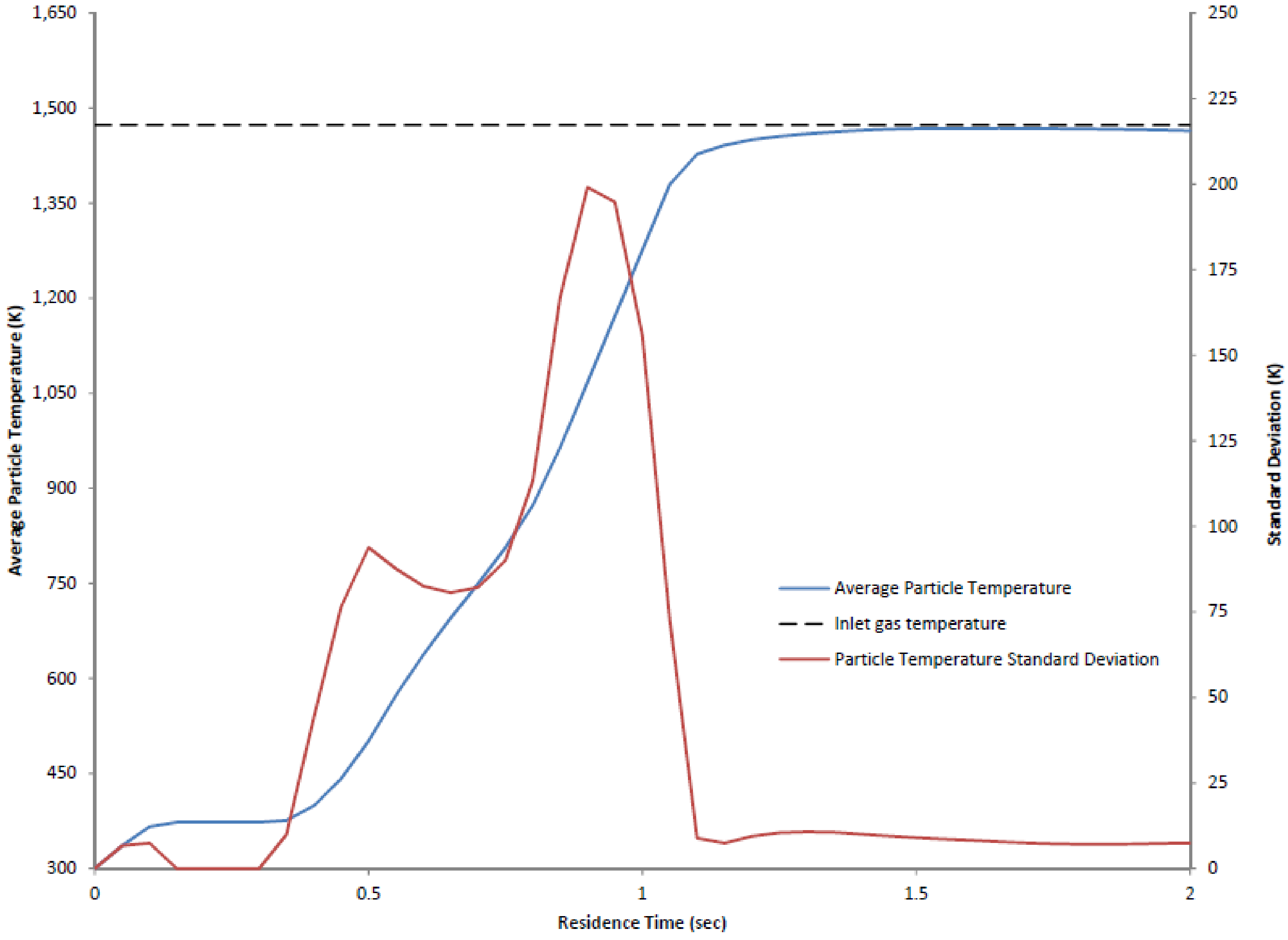
Fixed Carbon:	0.3545
Volatiles:	0.2910
Moisture:	0.2648
Ash:	0.0897

Ultimate Analysis:

Carbon:	0.4985
Hydrogen:	0.0340
Oxygen:	0.0950
Nitrogen:	0.0080
Sulfur:	0.0100

Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



Work Flow: Run CFD with C3M Chemistry

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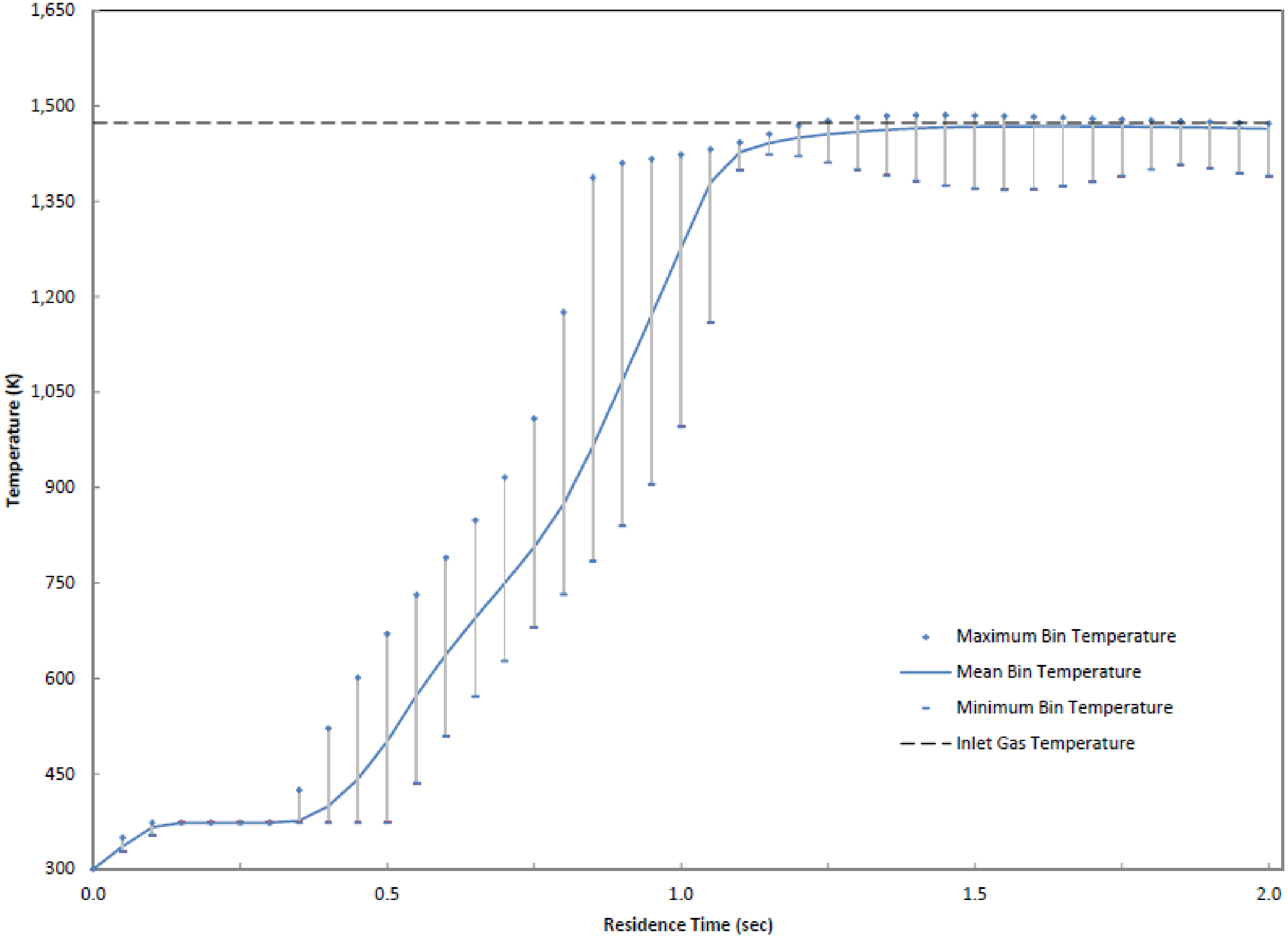

Work Flow: Run CFD with C3M Chemistry

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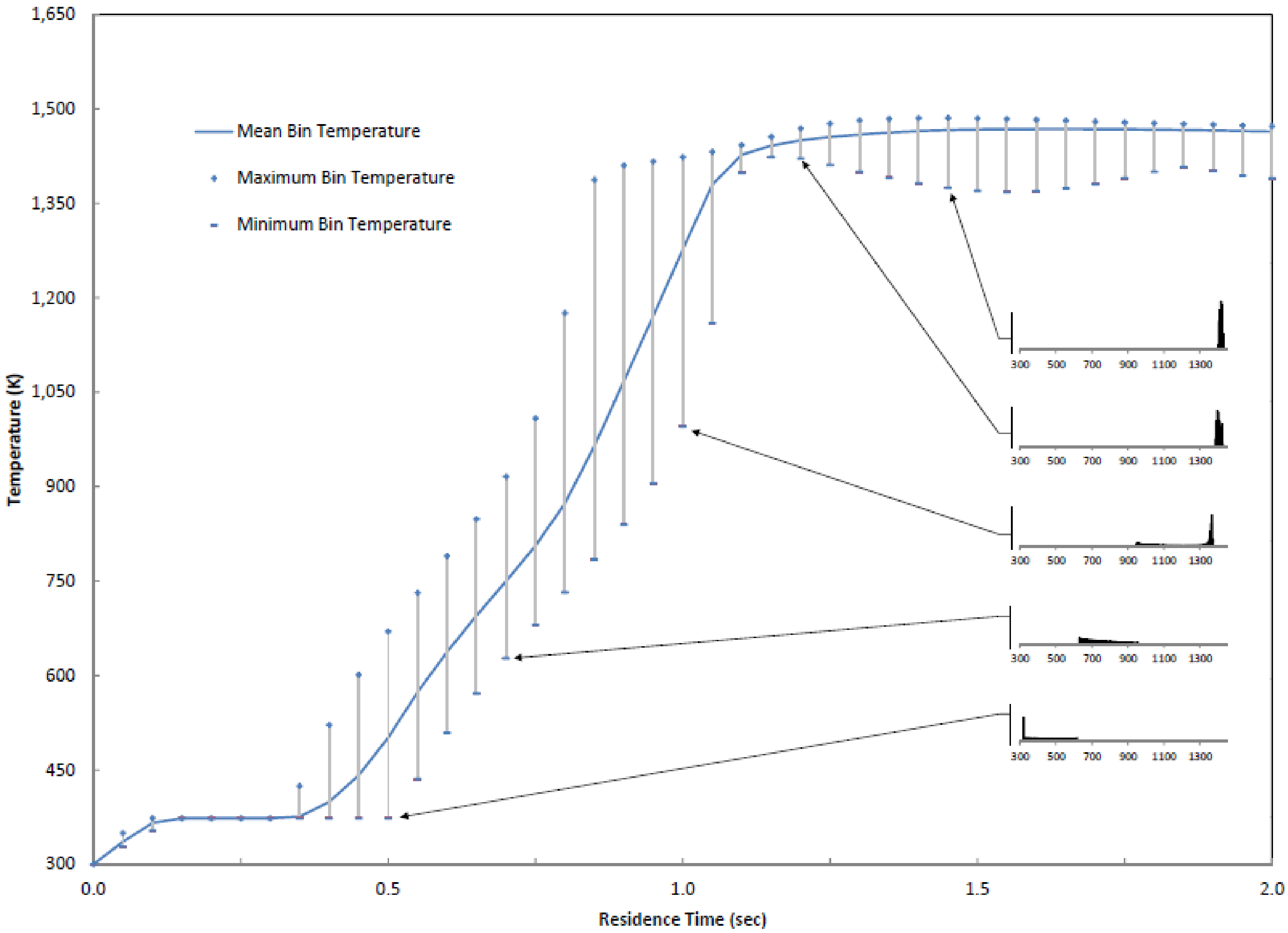
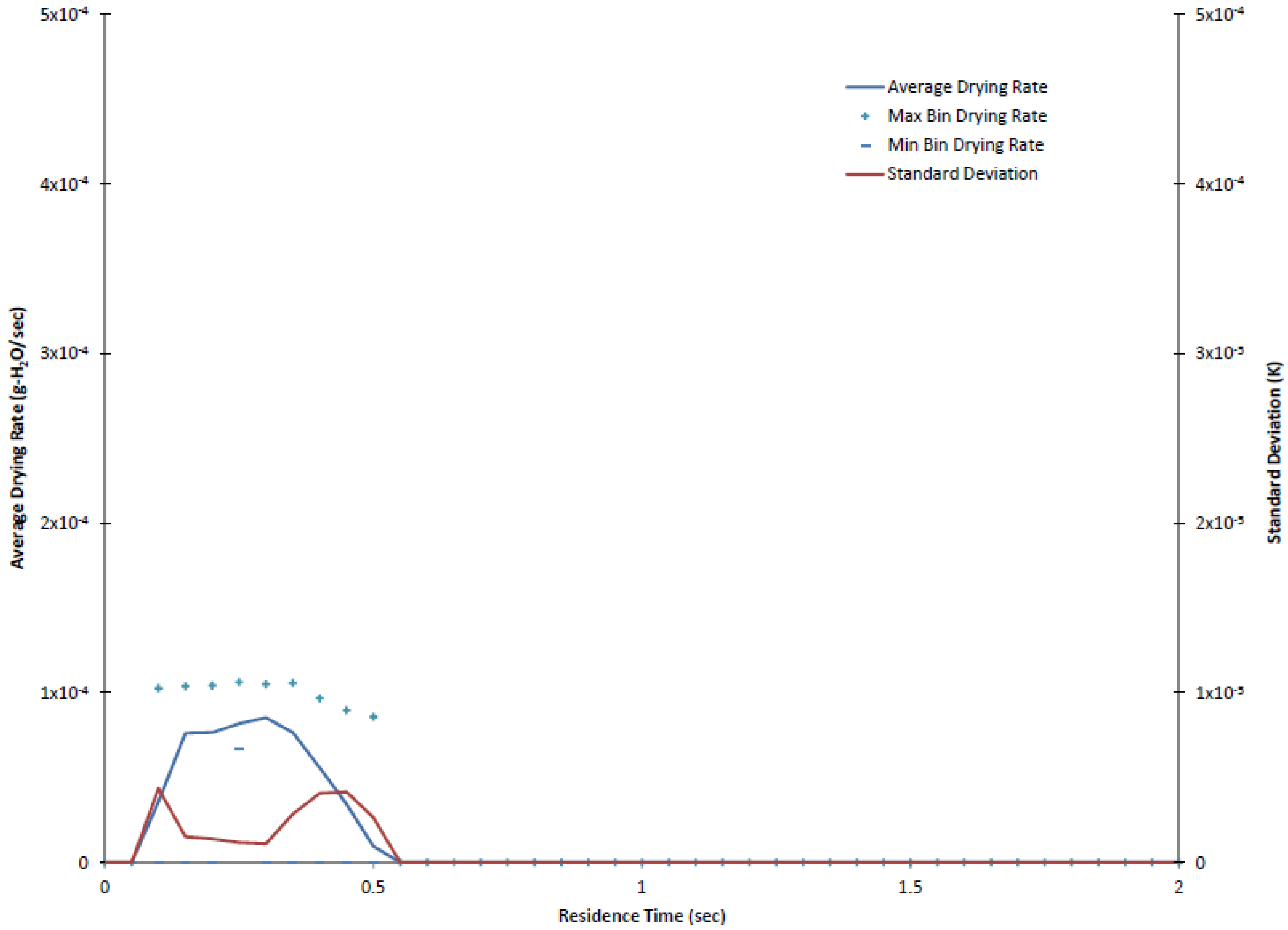


Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



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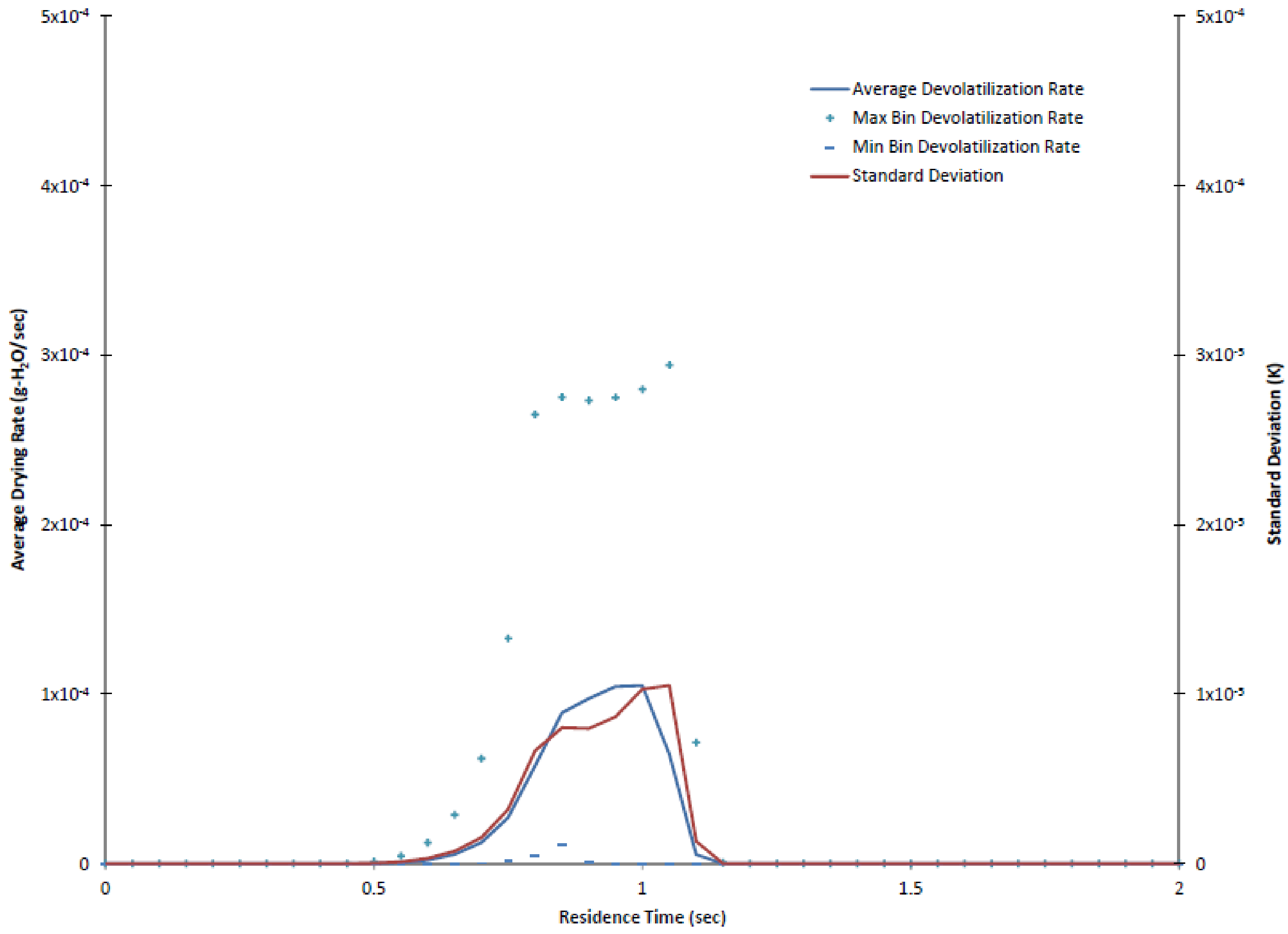
Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



Work Flow: Run CFD with C3M Chemistry

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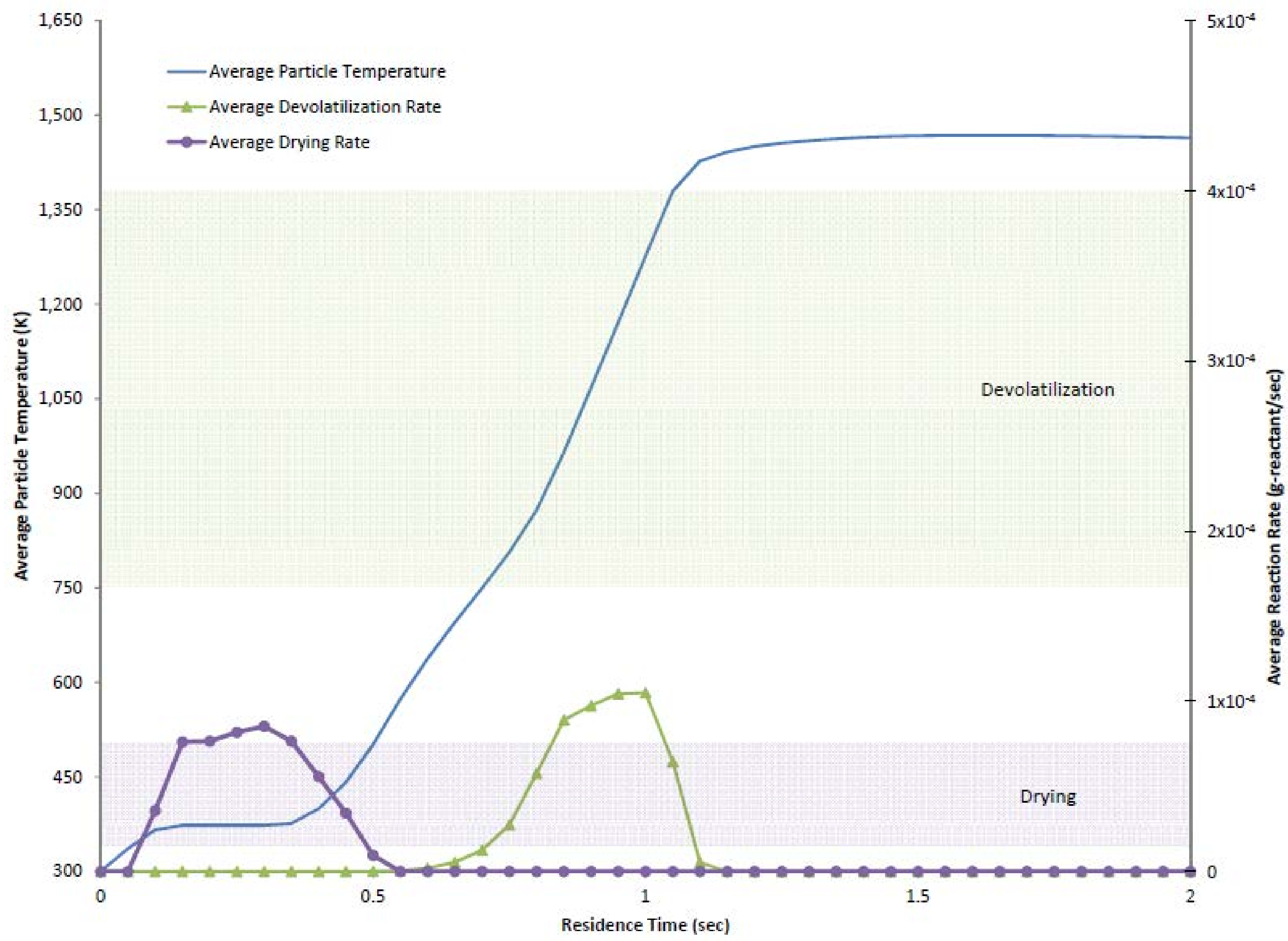
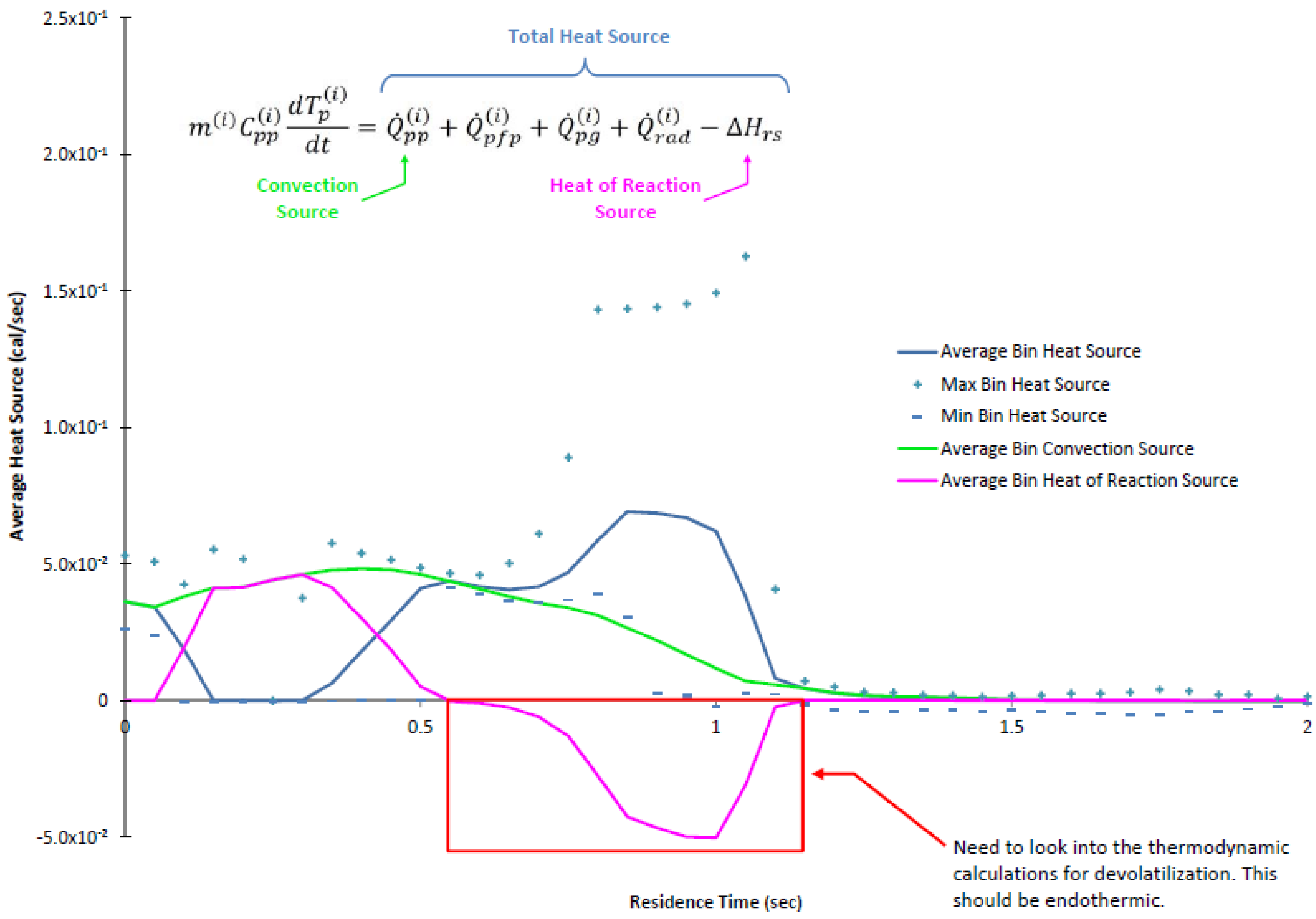


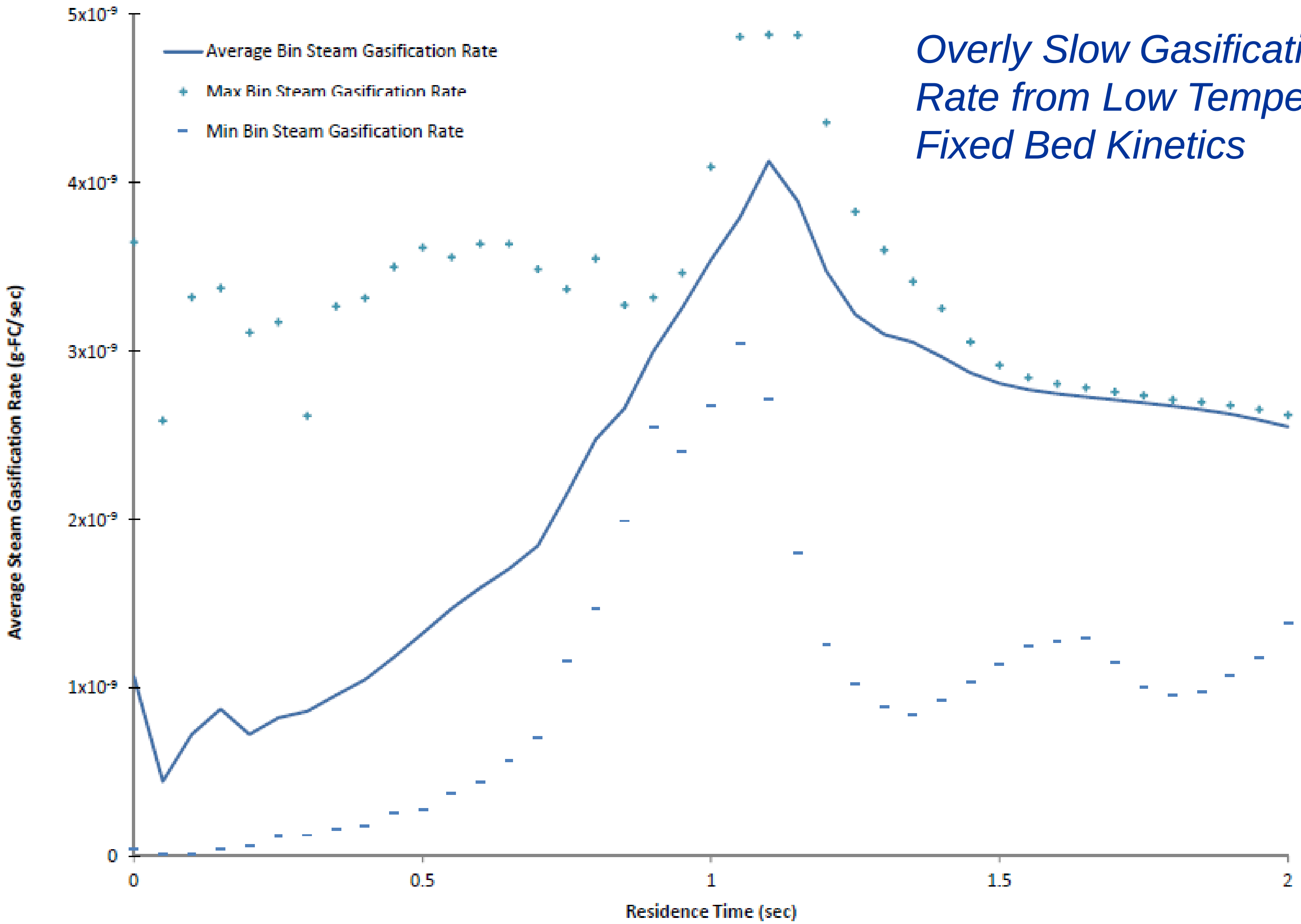
Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



Work Flow: Run CFD with C3M Chemistry

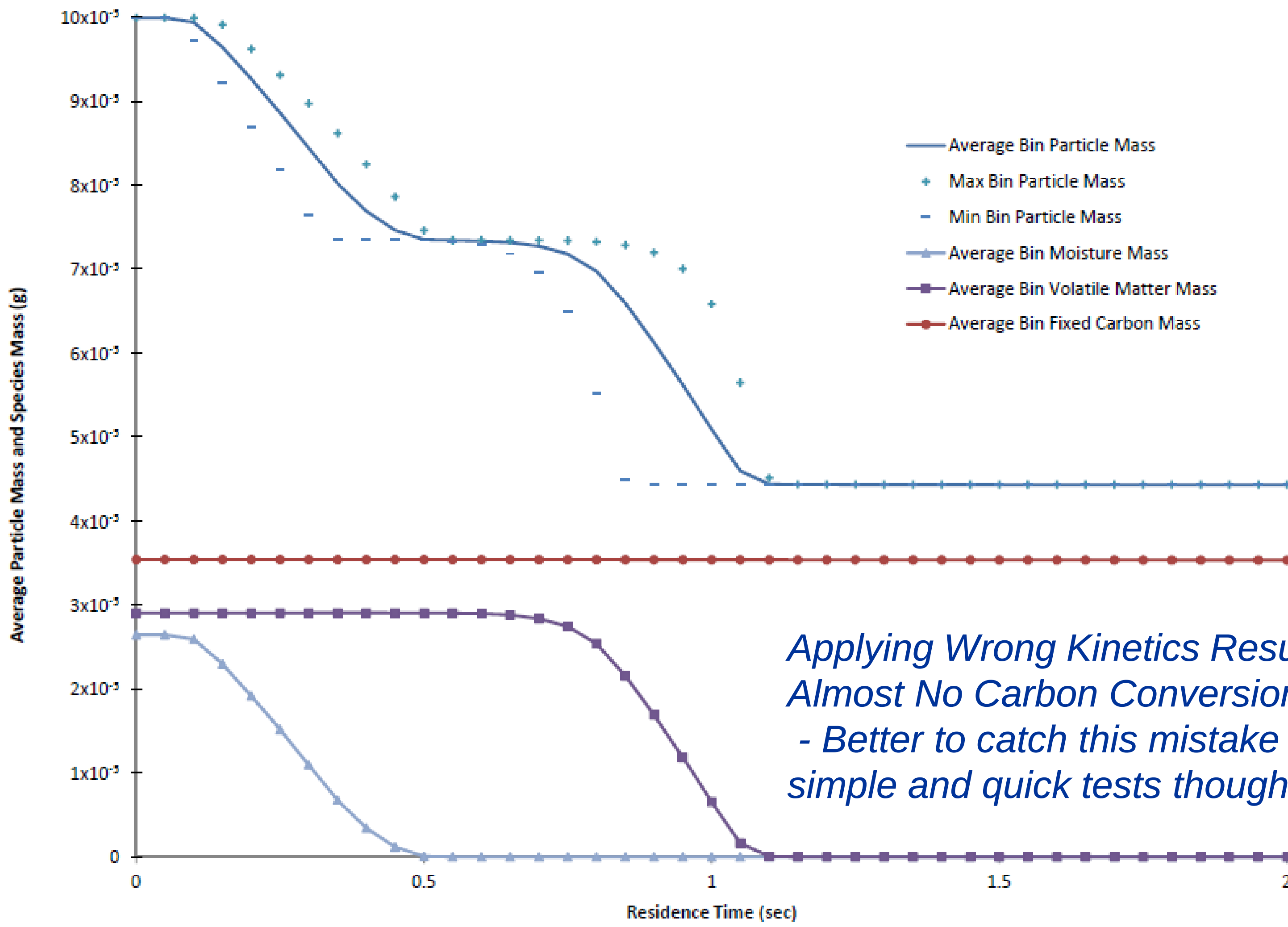
Example: Virtual Drop Tube Run in MFIX-DEM



Overly Slow Gasification Rate from Low Temperature Fixed Bed Kinetics

Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



Applying Wrong Kinetics Resulted in Almost No Carbon Conversion
- Better to catch this mistake early with simple and quick tests though C3M!

Why is C3M Needed?

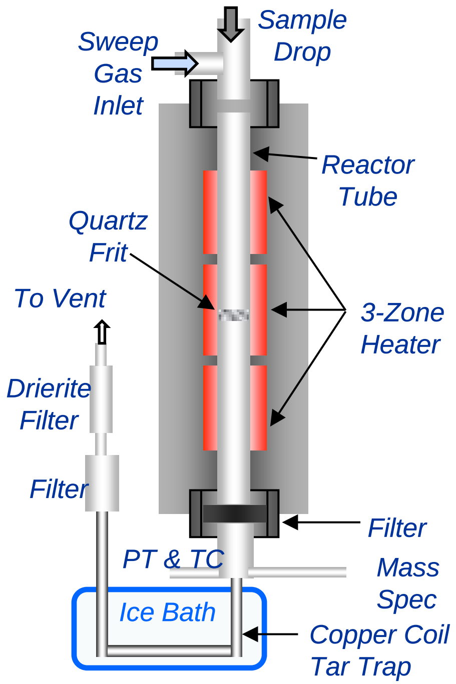
1. **Multiphase chemistry is complex (especially gasification)**
   - Real world chemistry can involve hundreds if not thousands of chemicals and reactions
   - Modelers simplify to as few as 10 or up to about 30 to capture major effects
2. **The literature availability is vast, searching for and applying kinetics is very time consuming**
3. **Not all kinetic expressions are suitable for or stable in CFD**
4. **Literature values are prone to error and have to be validated**
5. **The process of gathering, implementing, testing, and validating kinetic expressions can cost a CFD practitioner upwards of 1000 man hours and several hundred computational hours**

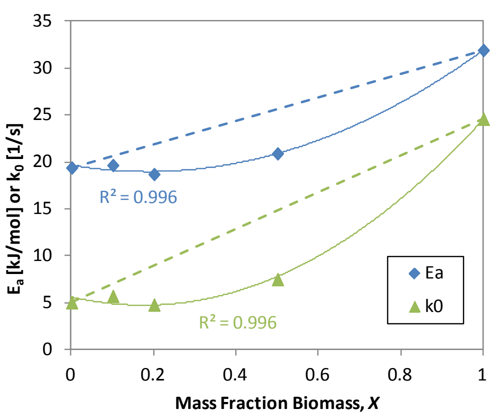
- **C3M can provide tested and validated kinetics to a CFD practitioner or researcher in minutes saving tremendous time and money in multiphase, reacting, CFD development**

What Does C3M Provide?

- **Direct links to kinetic data sources termed "Kinetic Packages" with appropriate licensing**
  - MGAS, PCCL, CPD, FG-DVC, and NETL HPTR Data
- **Chemical expressions and kinetic rates for gasification**
  - Moisture Release
    - Sources: MGAS and PCCL
  - Pyrolysis (Primary, Secondary, and Tar Cracking)
    - Sources: MGAS, PCCL, CPD, FG-DVC, and NETL HPTR Data
  - Char Gasification
    - Sources: MGAS and PCCL
  - Soot Gasification
    - Sources: PCCL
  - Water-Gas-Shift
    - Sources: MGAS
  - Gas Phase Combustion
    - Sources: MGAS
  - Char Oxidation
    - Sources: MGAS and PCCL
  - Soot Oxidation
    - Sources: PCCL
  - Tar Oxidation
    - Sources: MGAS
- **Thermodynamic data for "Pseudo Species"**
- **Fuel Composition to be used in CFD (fixed carbon, volatile matter, moisture, and ash)**
  - Note: the information is similar to the proximate analysis for a fuel but determined under different heating rates and temperatures than the standard test, so the values may be different
- **Graphical plots showing product composition and rates**
- **A comprehensive report detailing all equations in the chemical system**
- **Formatted input files for ANSYS FLUENT, CPFD BARRACUDA, and NETL's MFIX**

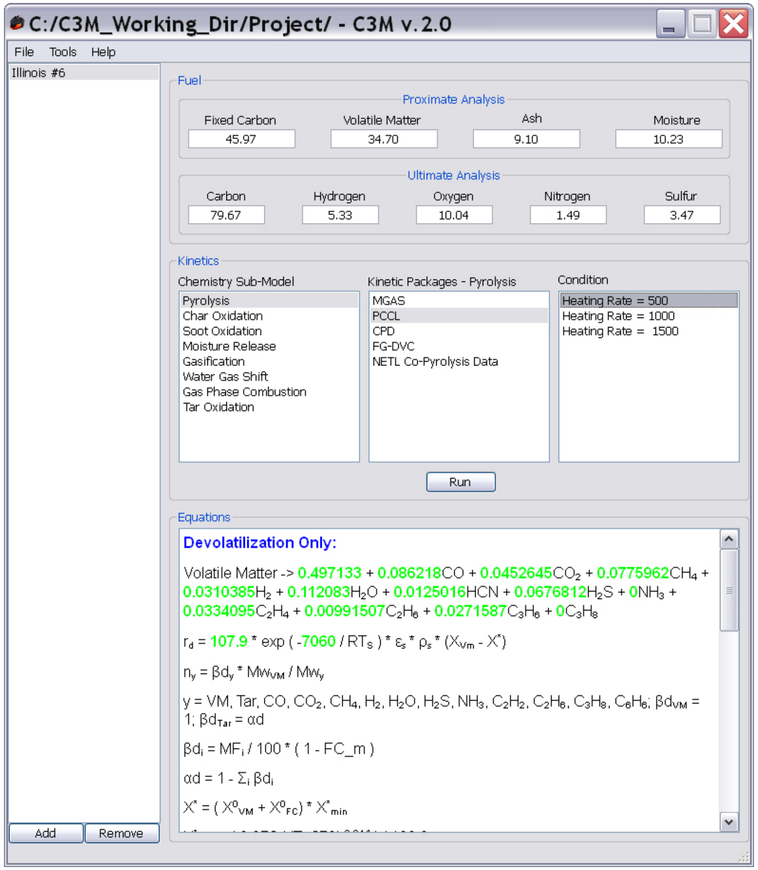
What Does C3M Provide?





- **Kinetic Data for Fuel Flexibility**
  - Completed test campaign for southern pine and PRB for co-pyrolysis
  - Found that product gas distributions vary linearly with biomass weight fraction but kinetic rates do not
  - Data analysis is complete and reduced to a functional module within C3M
  - Testing is under way for co-gasification kinetics

What Does C3M Provide?



- **Easy, Intuitive, Reliable, and Graphical User Interface**
  - No cryptic text based systems
  - Intuitive work flow
  - Easy data visualization
  - Speed in building complex chemistry models
  - Reliable and tested sources of information