



NATIONAL ENERGY TECHNOLOGY LABORATORY



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

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August 6, 2013 – NETL Multiphase

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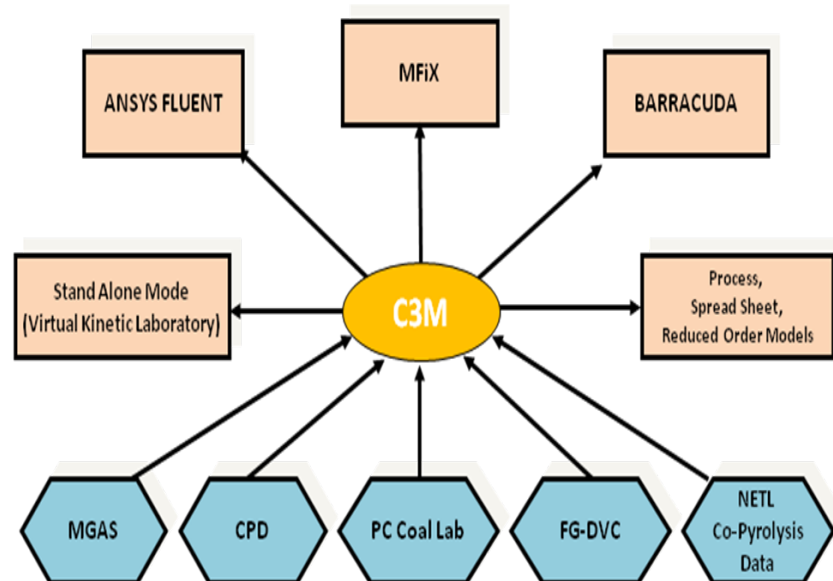
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Richard Turton, WVU
Nathan Weiland, WVU
Nicolas Means, WVU



What is C3M

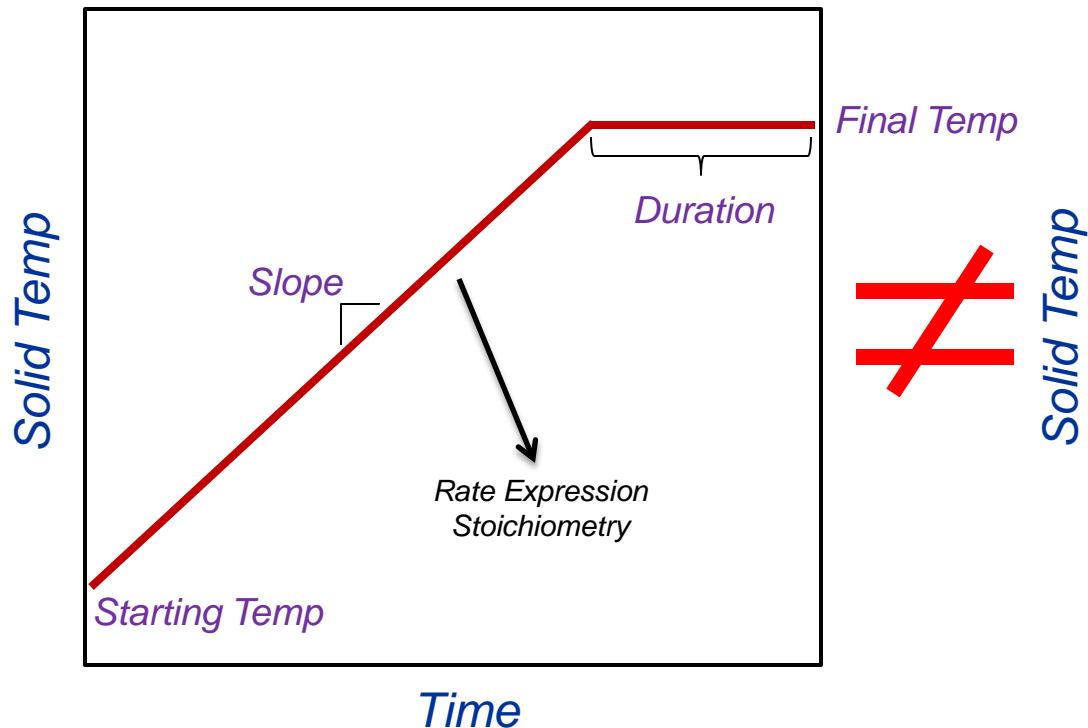
- **Chemical Kinetics Management Software**

- 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

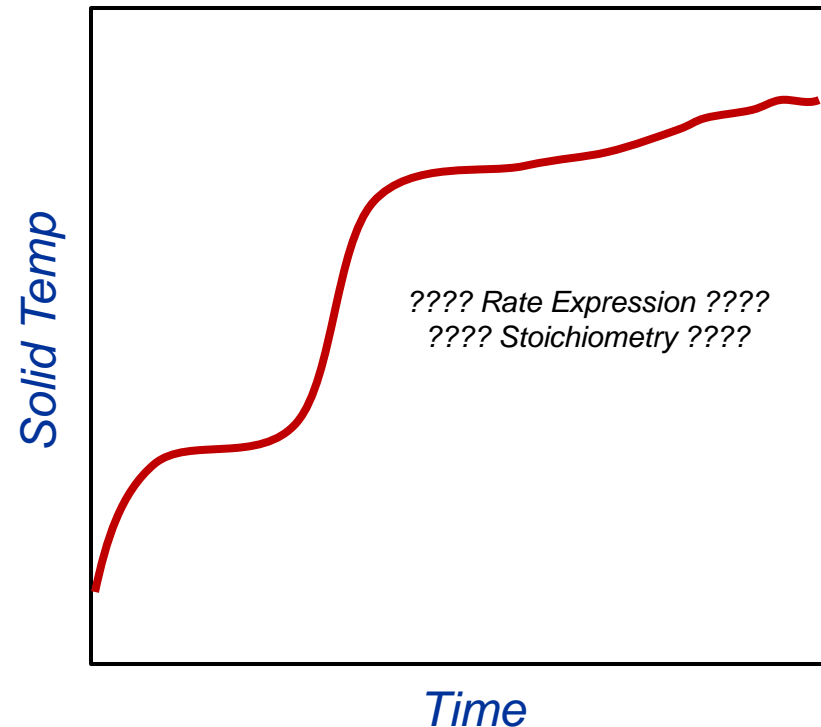


Motivation

Prescribed Sub-Model Test



Real/Modeled World

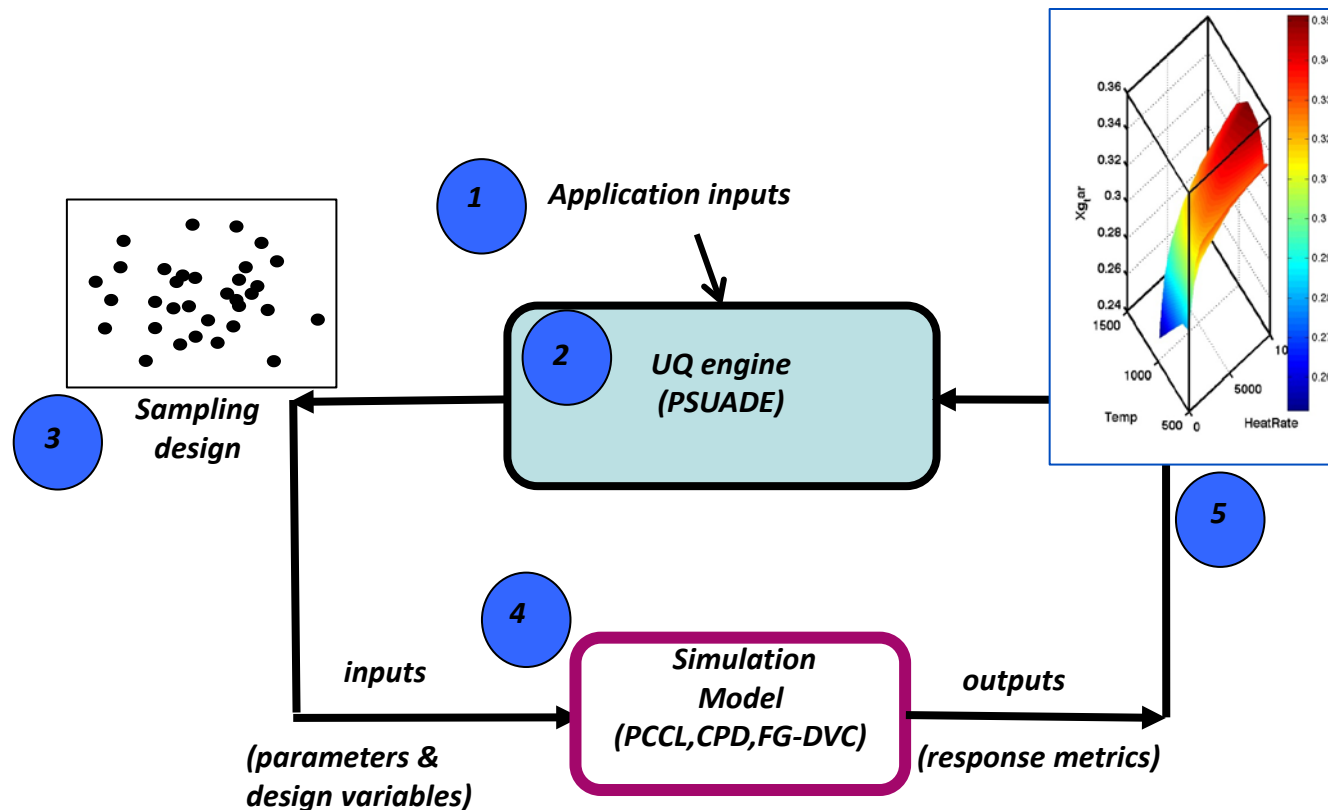


- **Current Focus: Devolatilization**
 - Uncertainty in Heating and Final Temp

Solution: Use Tools from UQ

Uncertainty Quantification

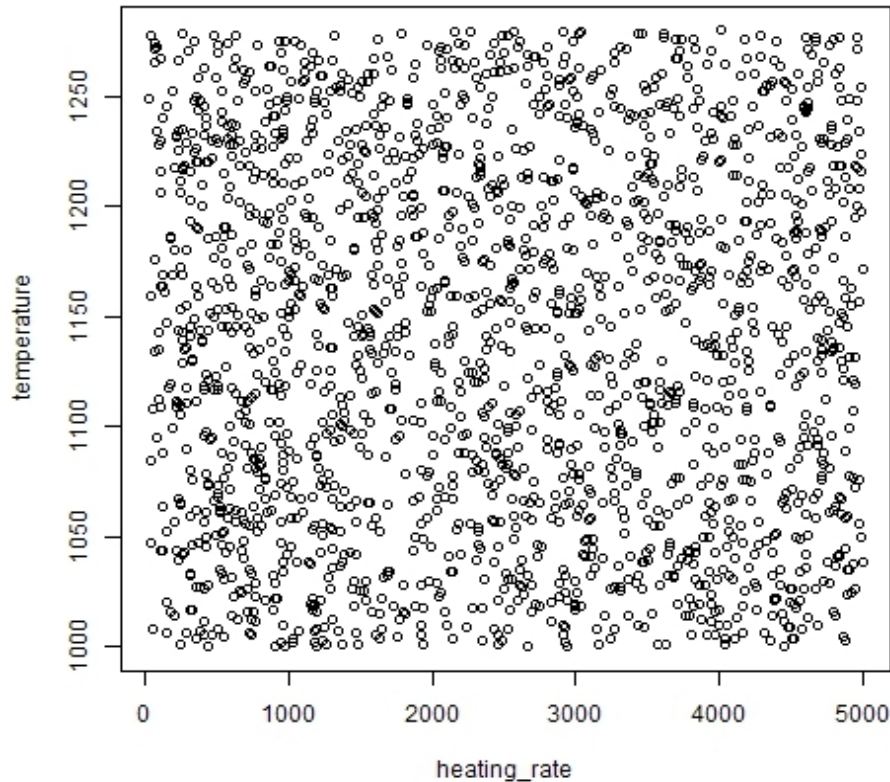
Input Uncertainty Propagation and Quantification (Non-intrusive method)



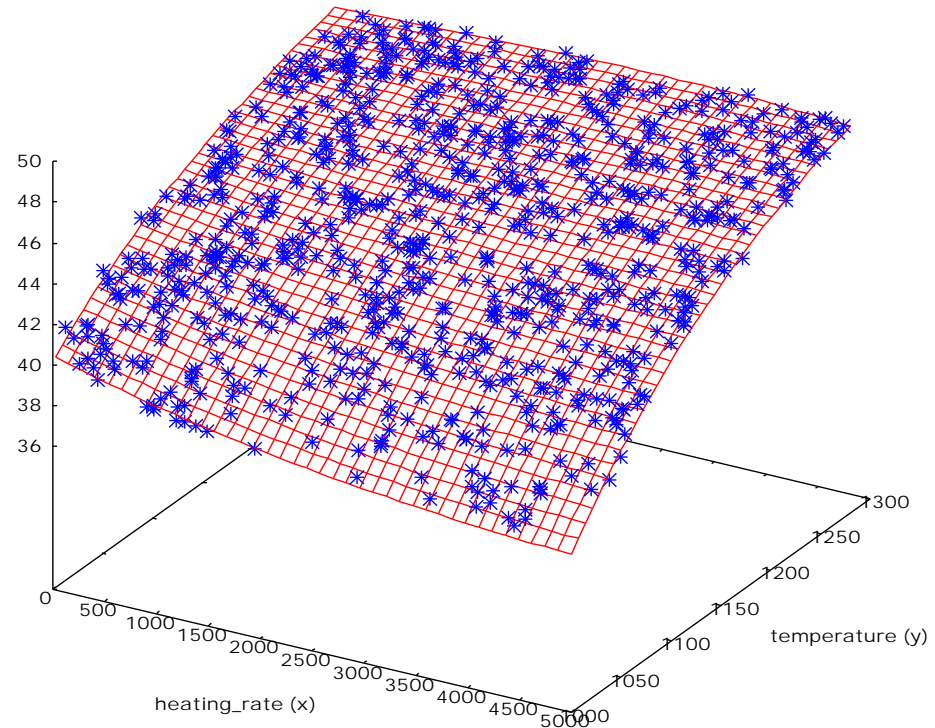
Solution: Use Tools from UQ

*Uncertainty Quantification
PCCL with PRB Example*

Sample Design Space

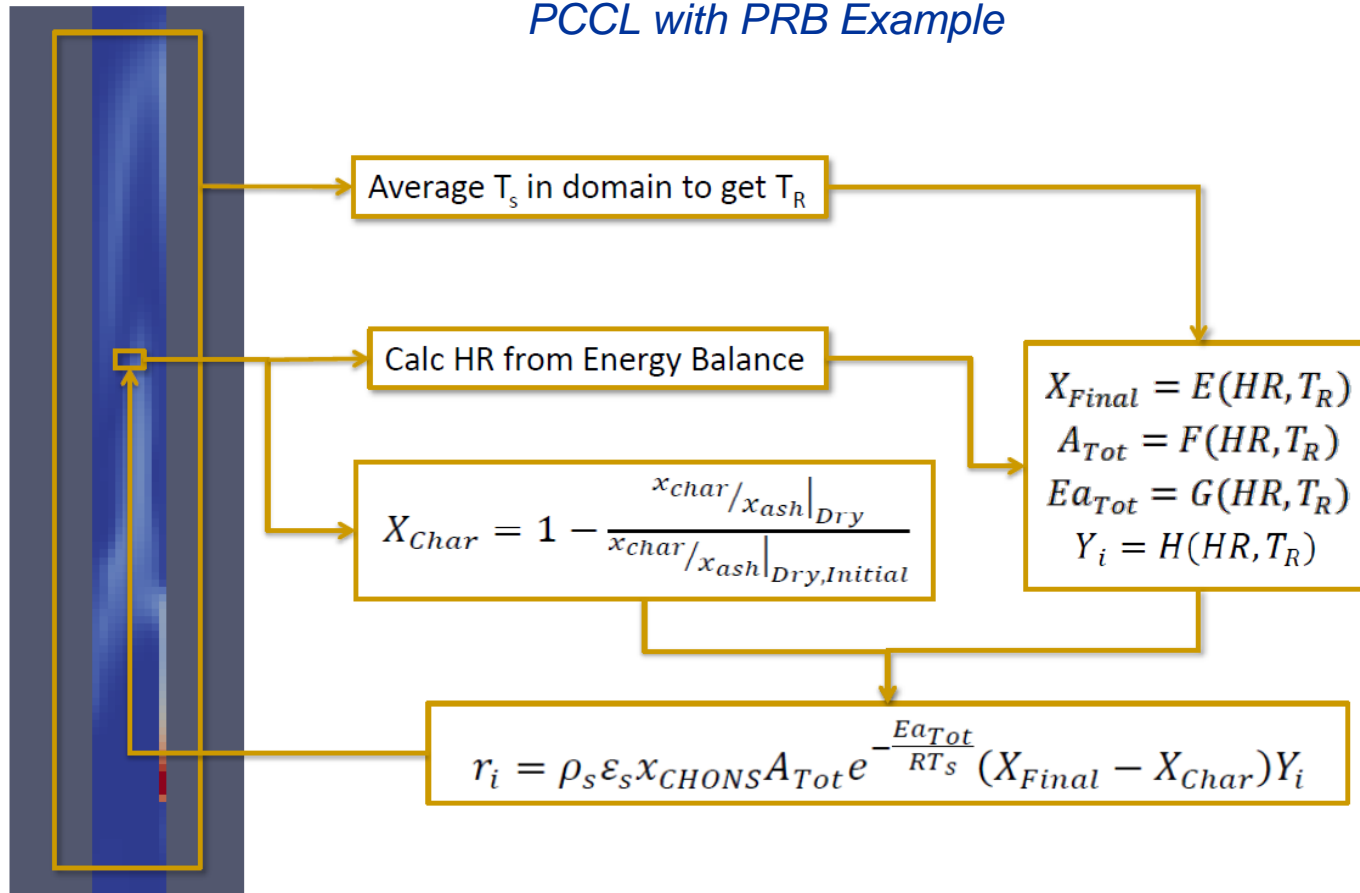


*Example Response Surface
Total Volatile Yield*

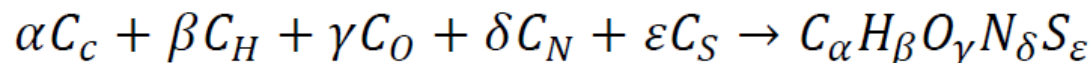


Solution: Use Tools from UQ

*Build Surrogate Model in CFD
PCCL with PRB Example*

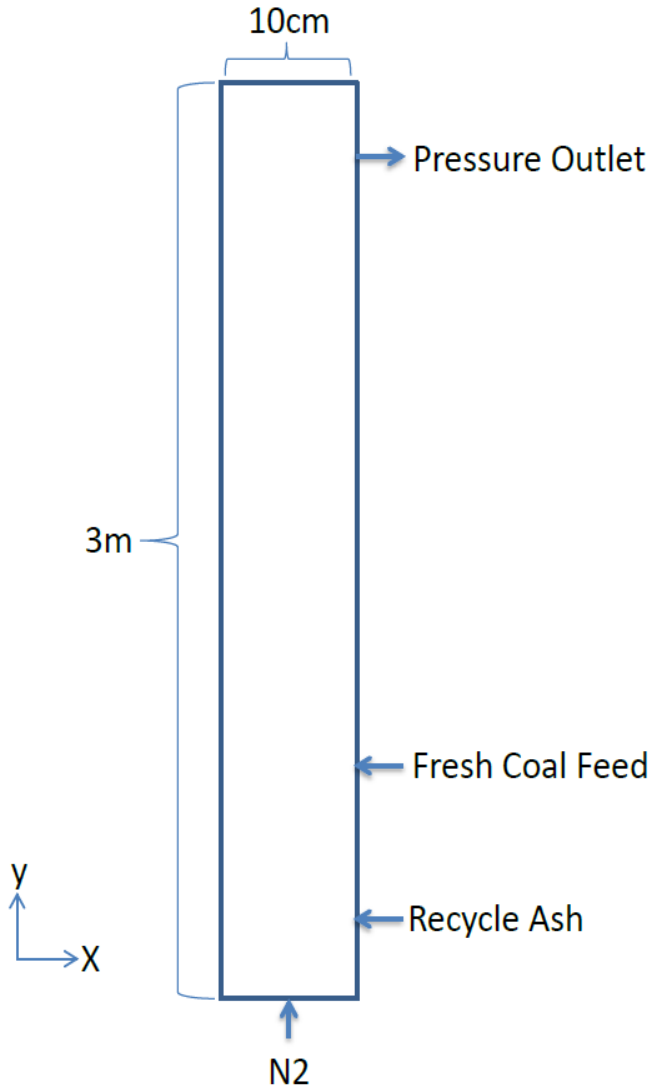


*7 component coal model: Ash Moisture, Carbon, Hydrogen, Oxygen, Nitrogen, Sulfur
Each gas formed during devolatilization has it's own chemical formula and rate:*



Example Test Case

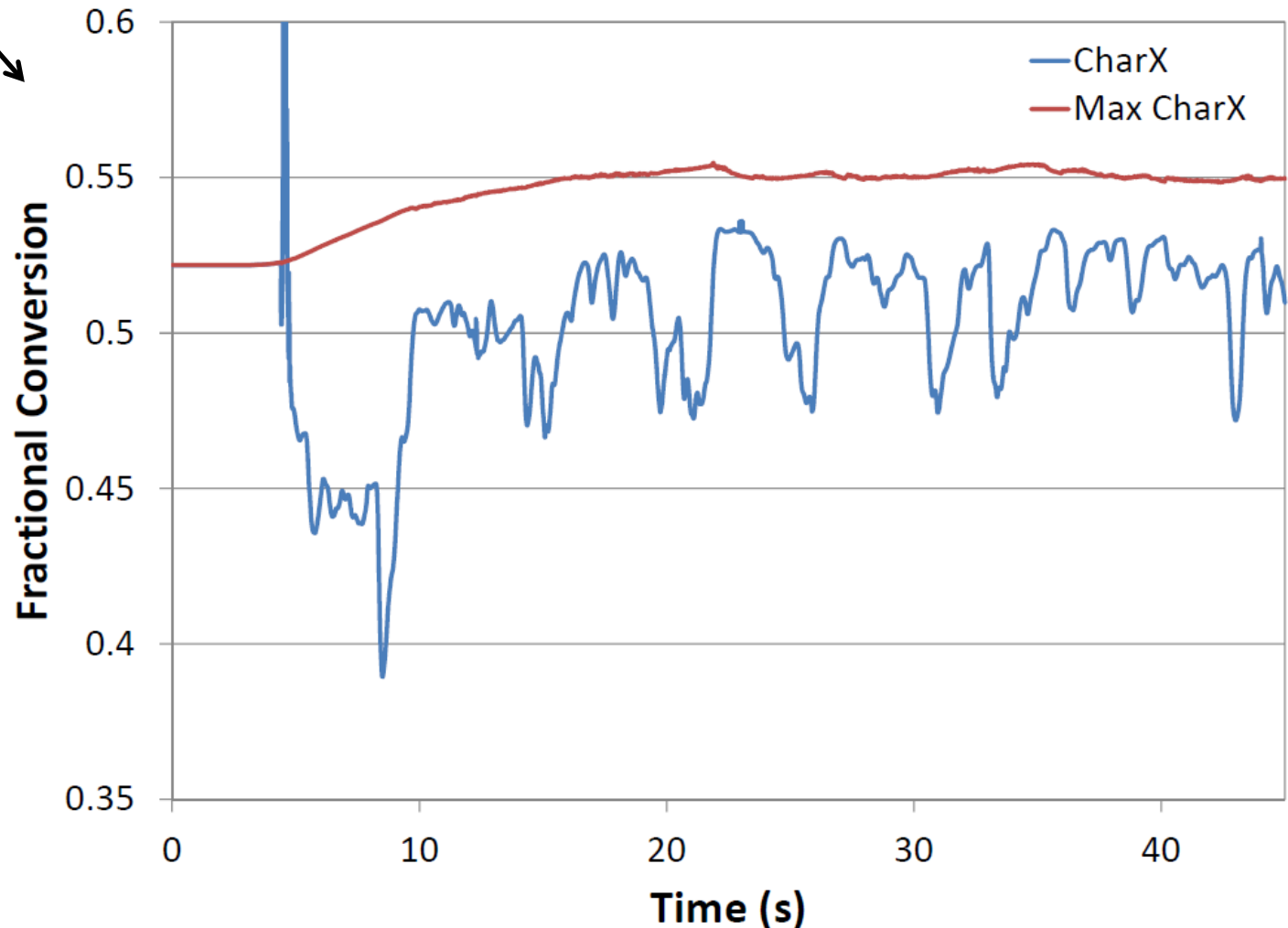
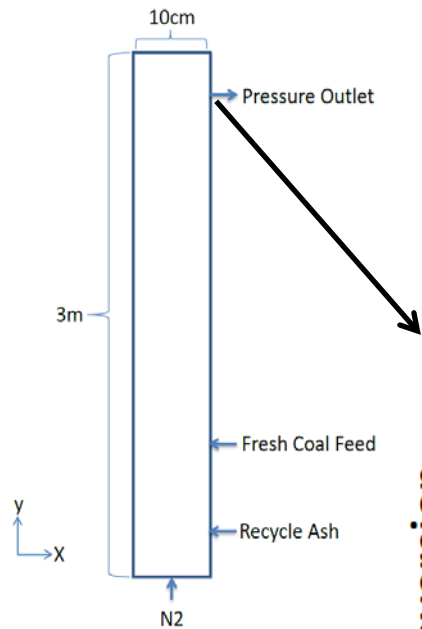
Pseudo 2D Transport Reactor



- **Grid: 10 x 320 (~1cm res)**
- **N₂/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

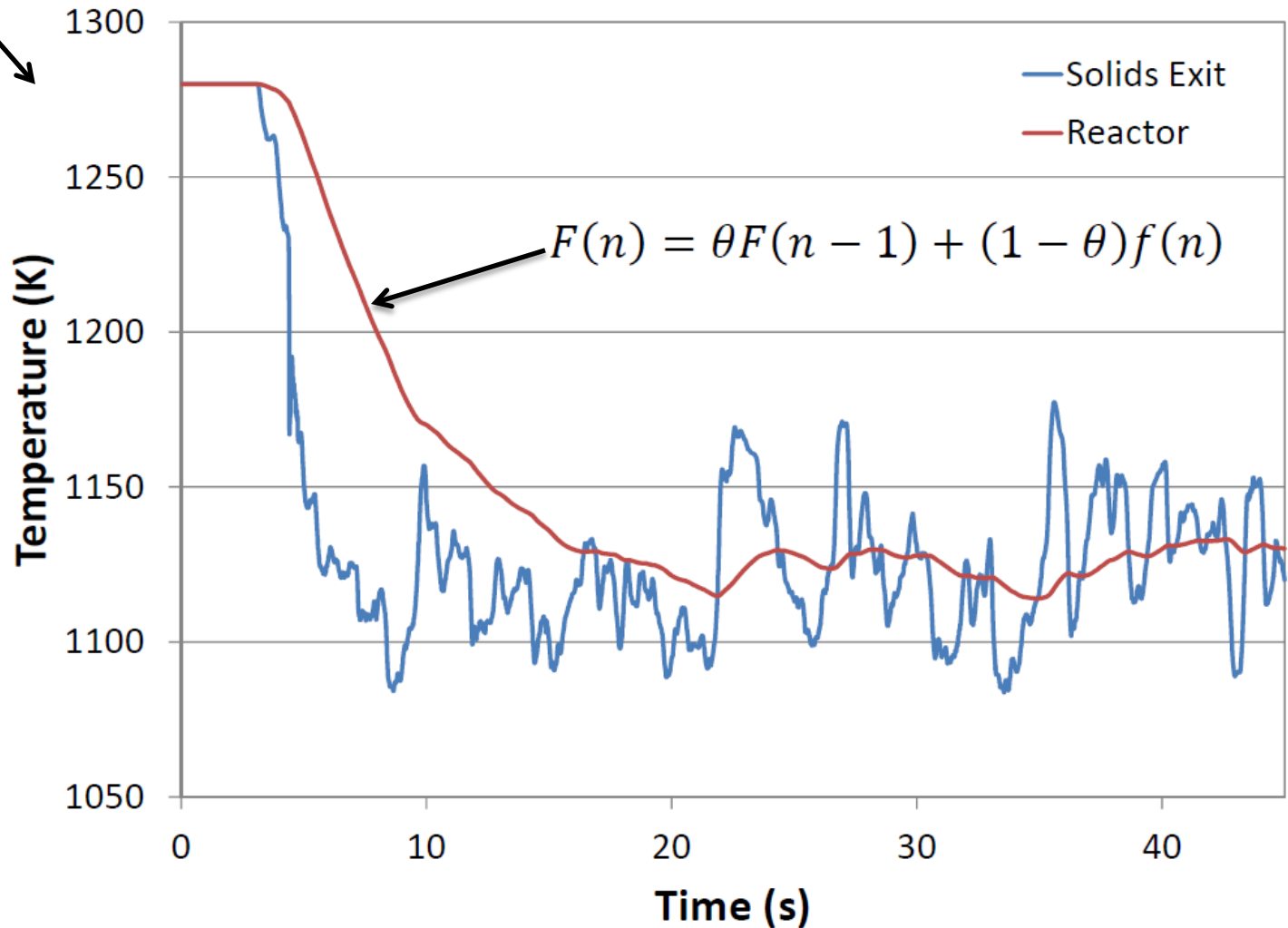
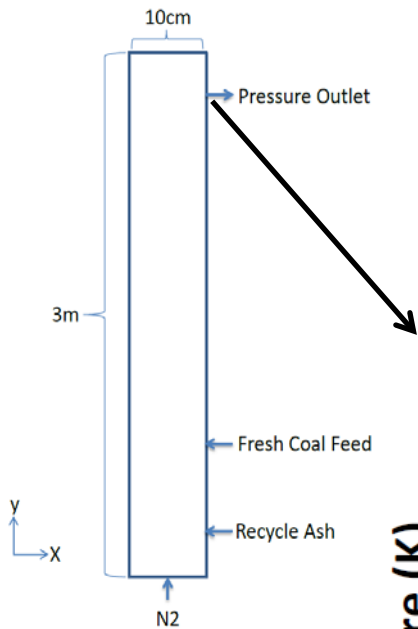
Coal Conversion at Exit



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

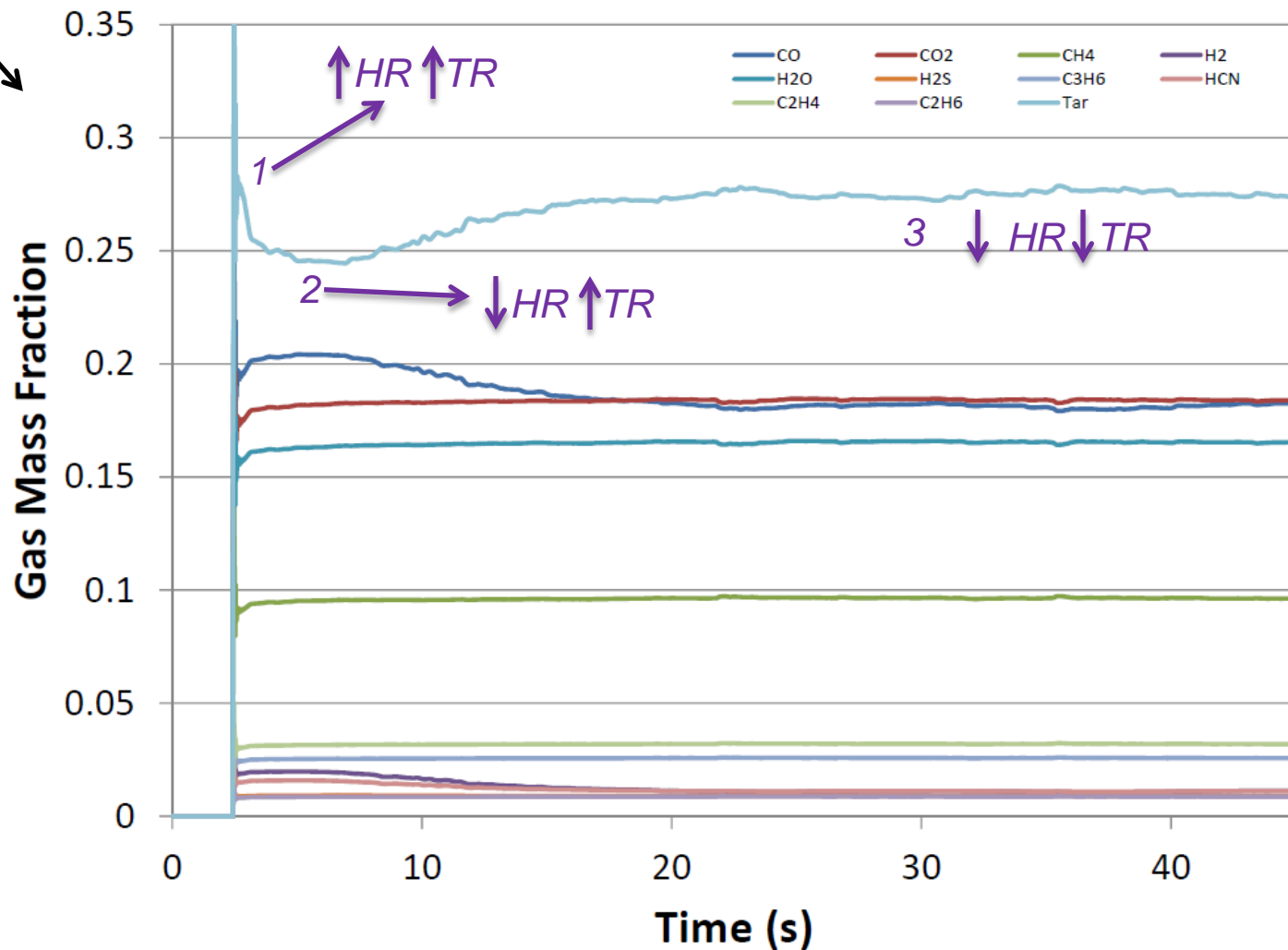
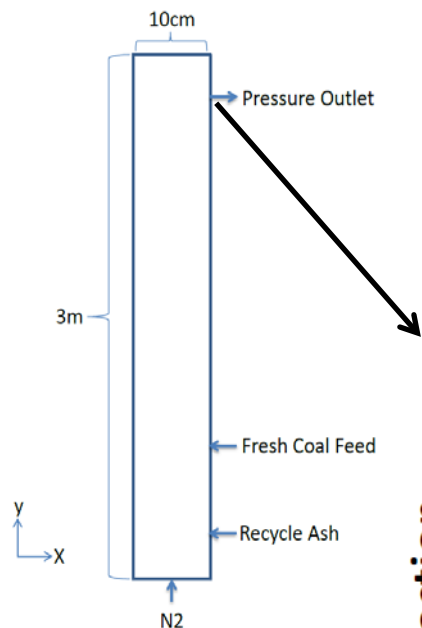


Reactor temp. is calculated by time filtering the solids temp. at the exit of the reactor

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

Example Test Case

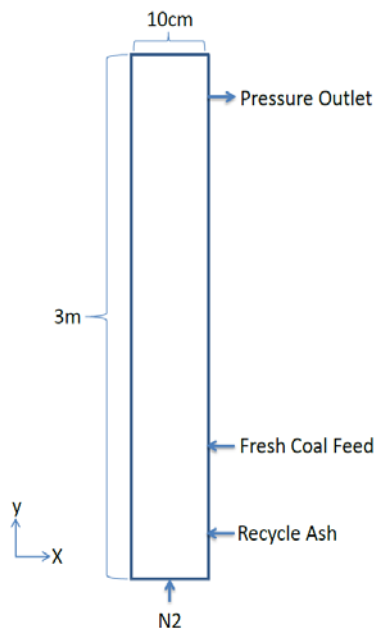
Fractional Product Yield, Mass Basis at exit



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

Heating rate falls quickly as solids cool the path to travel

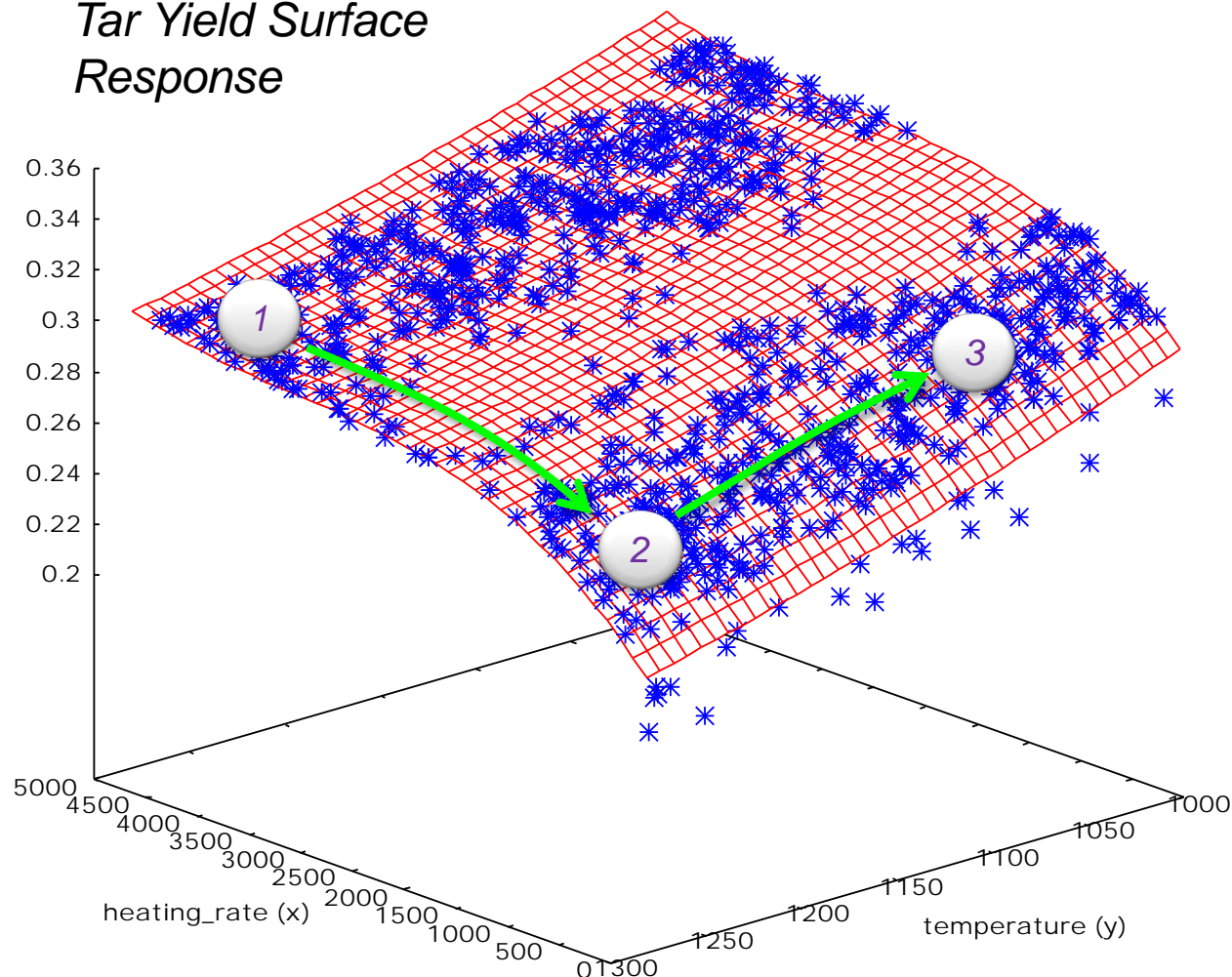
Cooler solids exit reactor and begin to set the reactor temp



Example Test Case

Understanding Product Yields

Tar Yield Surface Response



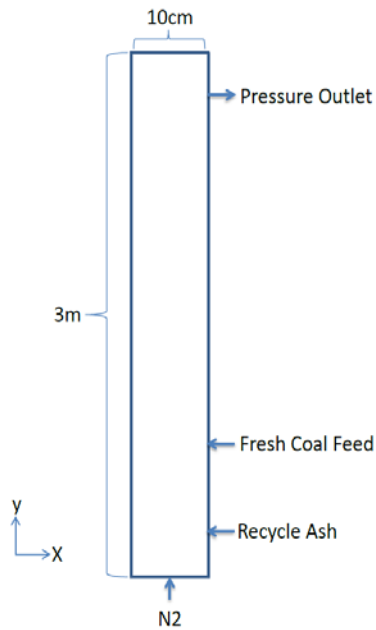
Initial heating rate is very high, and calculated reactor temp is high

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

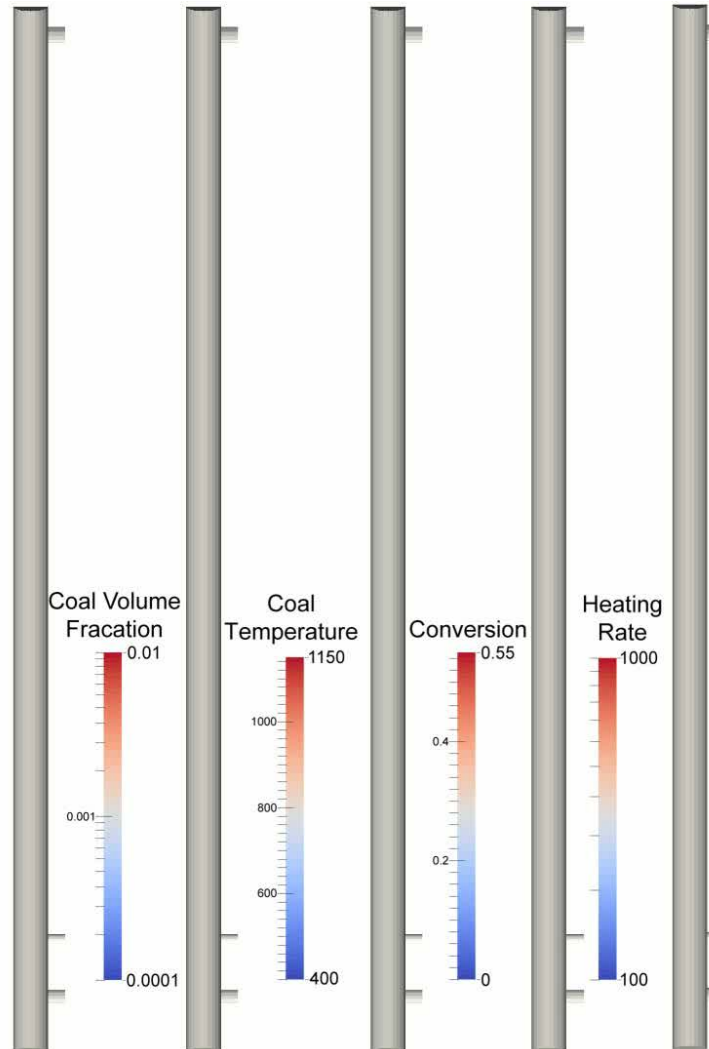
Understanding Product Yields



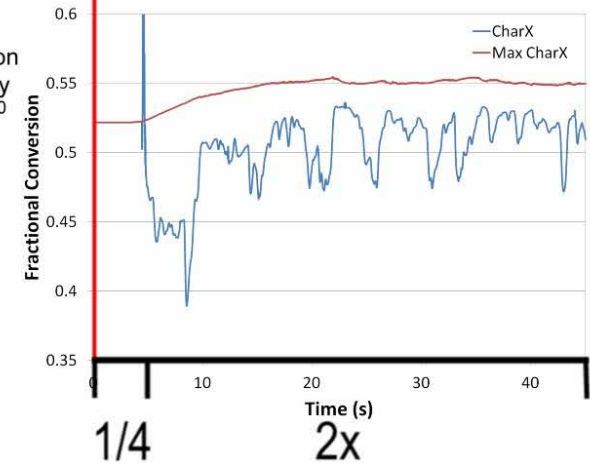
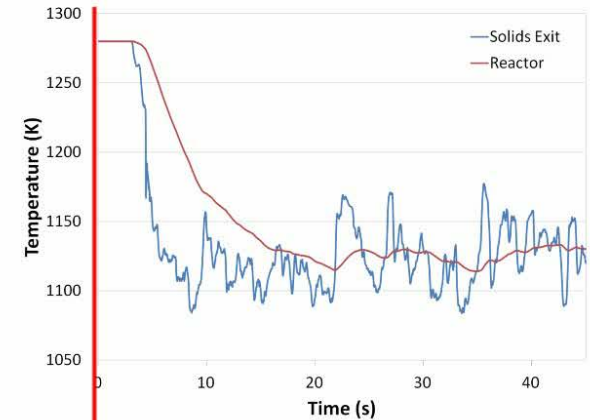
Initial heating rate is very high, and calculated reactor temp is high

Heating rate falls quickly as solids cool the path to travel

Cooler solids exit reactor and begin to set the reactor temp



Time: 0.0000

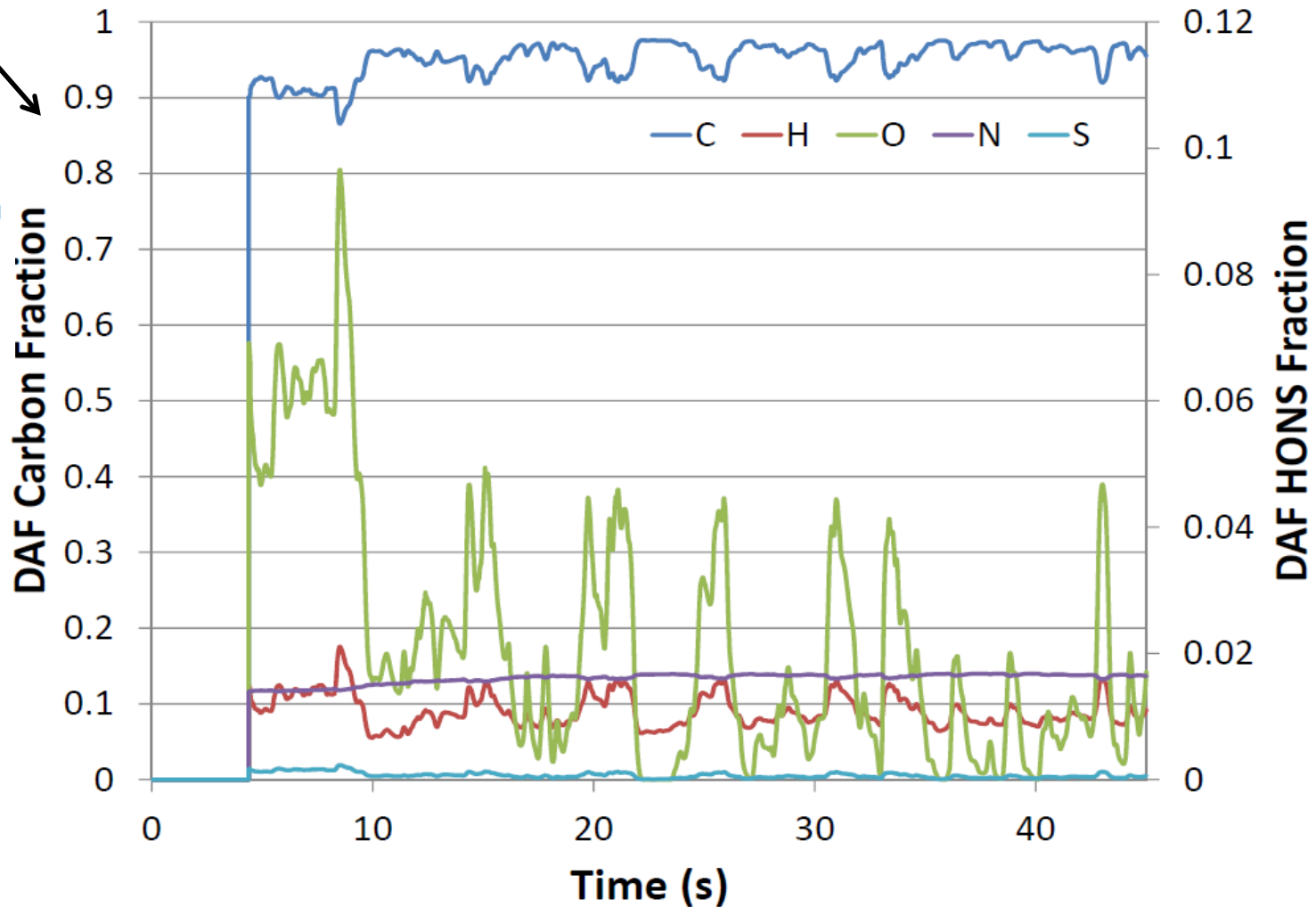
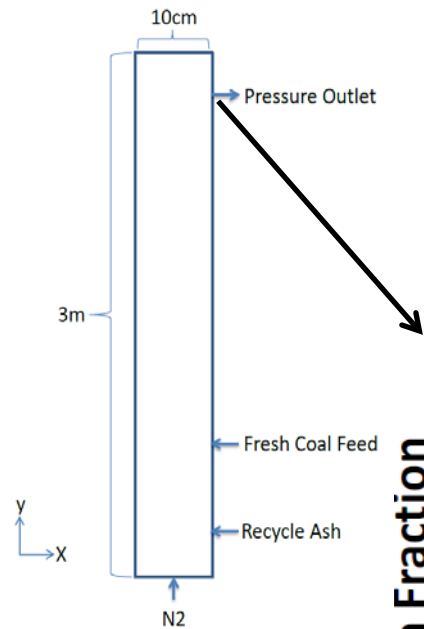


1/4

2x

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://mfex.netl.doe.gov/members/download_C3M.php

Thank You for Your Attention!

Reserve Slides

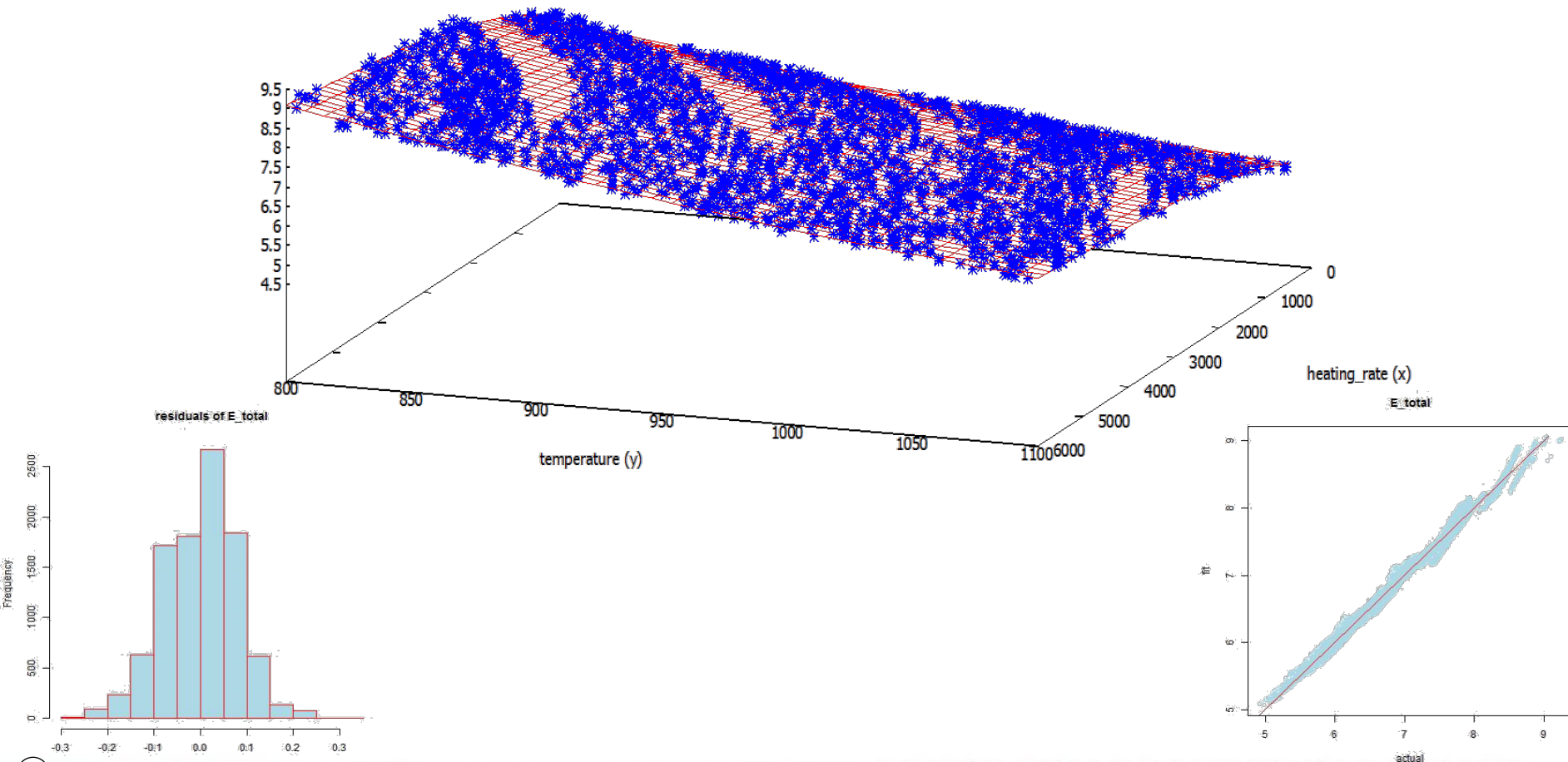
What's New in C3M?

Surface Response Modeling with CHONS Coal

PCCL with PRB Example

E_{total} [adjusted $R^2 = 0.99111$]

$17.761 + 0.0019267 * x - 1.7205e-007 * x * x + 1.0137e-011 * x * x * x + 2.8015e-011 * x * x * y - 1.7537e-006 * x * y + 6.2122e-010 * x * y * y - 0.018678 * y + 6.0571e-006 * y * y + 1.2963e-010 * y * y * y$ —
'summary_for_r.txt' every 2::2 u 1:2:5 *



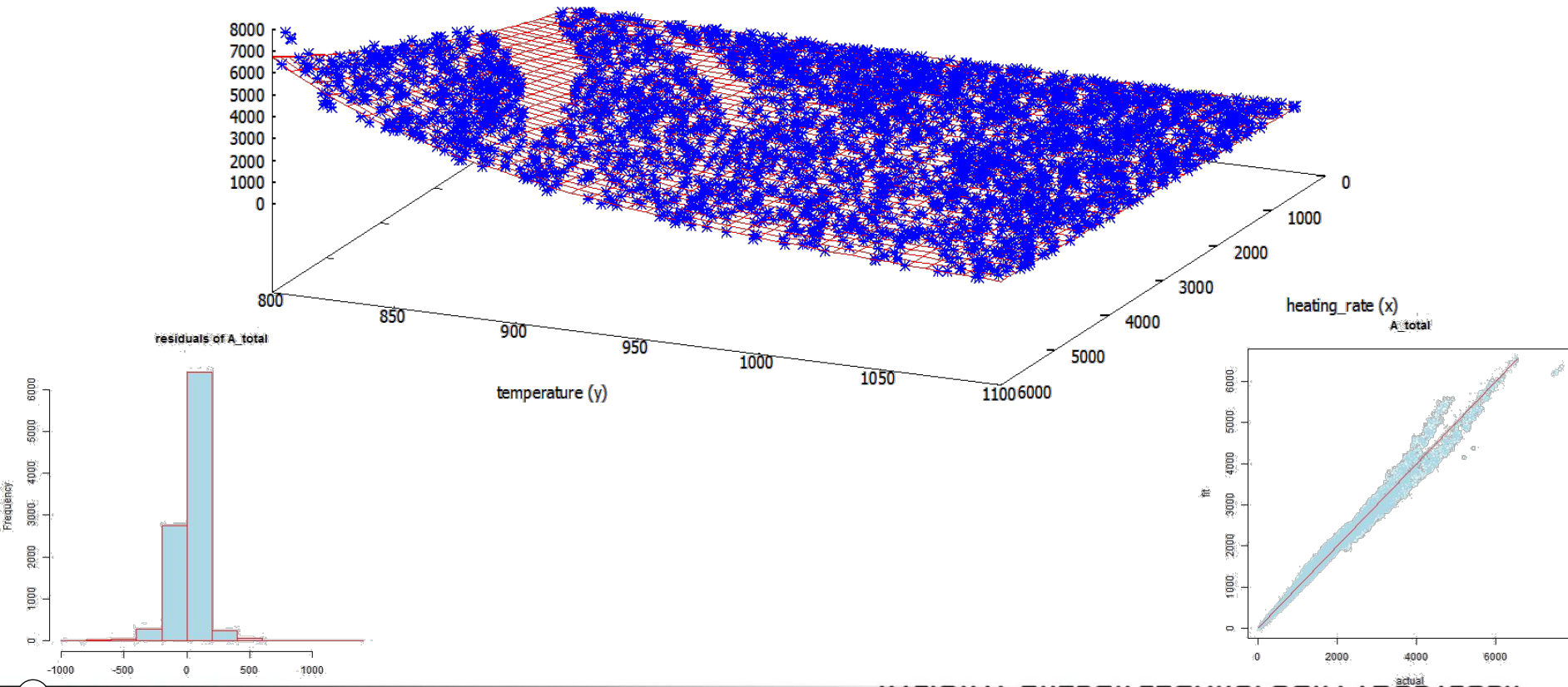
What's New in C3M?

Surface Response Modeling with CHONS Coal

PCCL with PRB Example

A_total [adjusted R² = 0.989776]

$(0.676448 * x + -38.9549) * 1.3369 * (0.00664942 * y + -3.2821) * -3.20472$ —
'summary_for_r.txt' every 2::2 u 1:2:4 *



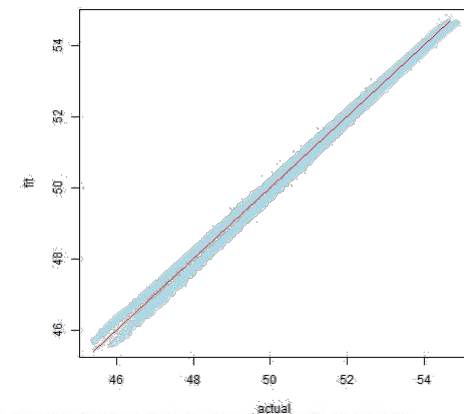
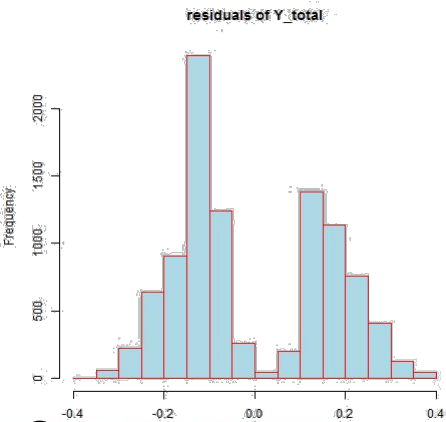
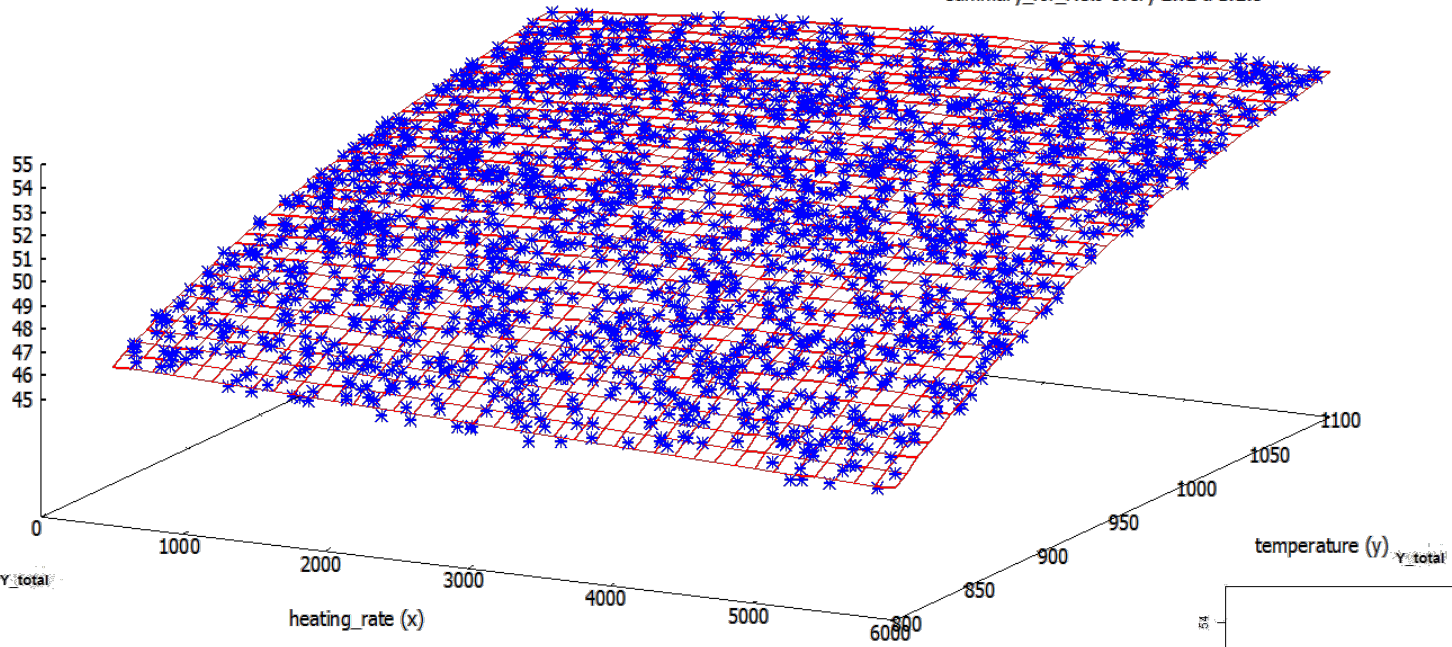
What's New in C3M?

Surface Response Modeling with CHONS Coal

PCCL with PRB Example

Y_{total} [adjusted $R^2 = 0.99468$]

$-111.98 - 0.0070278 * x + 1.1109e-007 * x^2 + 5.6659e-012 * x^3 - 2e-010 * x^4 + 1.2813e-005 * y - 5.2187e-009 * y^2 + 0.43719 * y^3 - 0.00039735 * y^4 + 1.2376e-007 * x * y$
'summary_for_r.txt' every 2::2 u 1:2:3 *



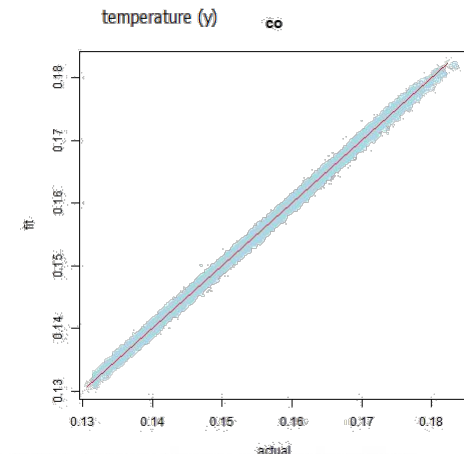
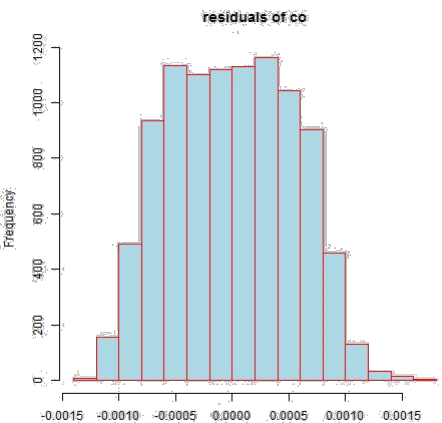
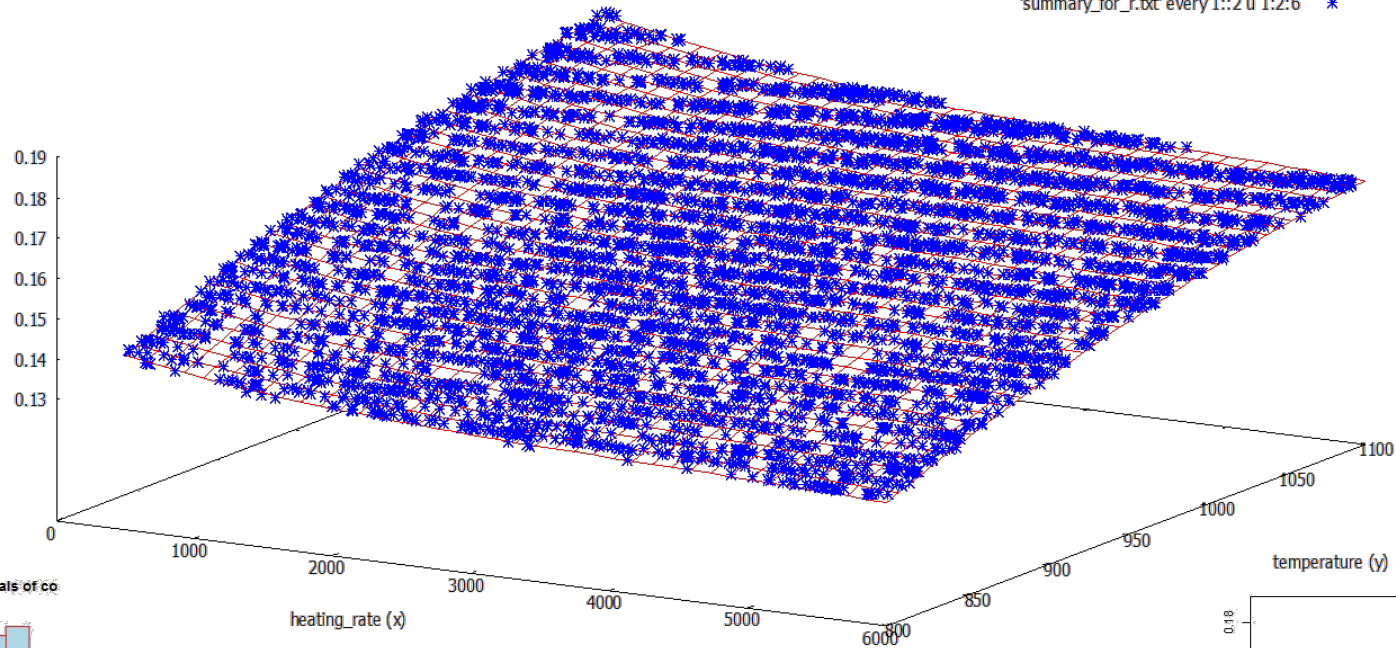
What's New in C3M?

Surface Response Modeling with CHONS Coal

PCCL with PRB Example

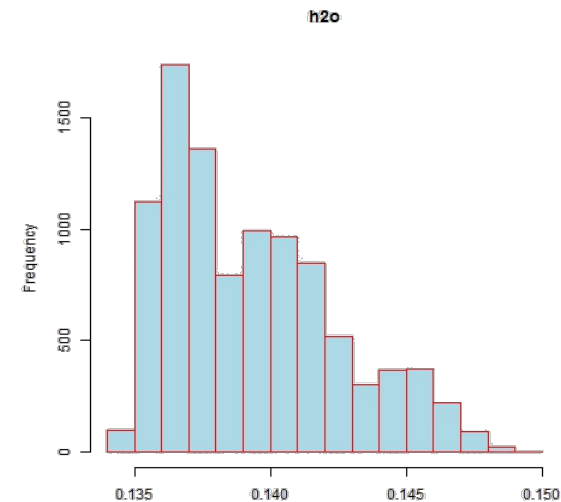
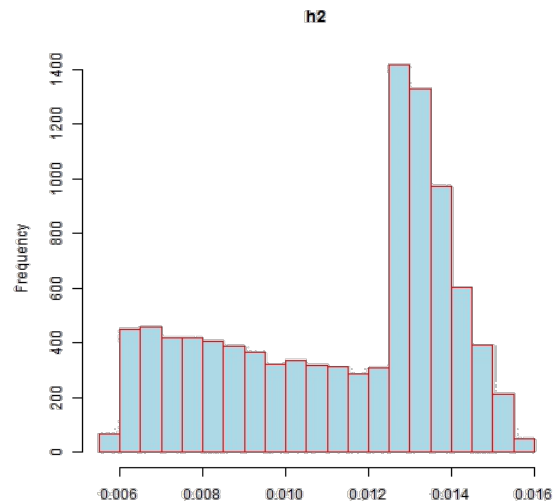
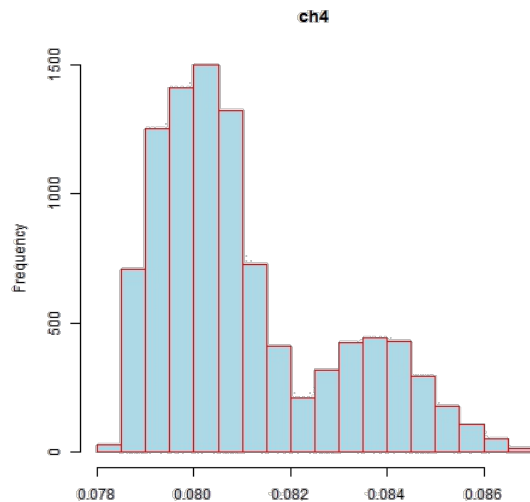
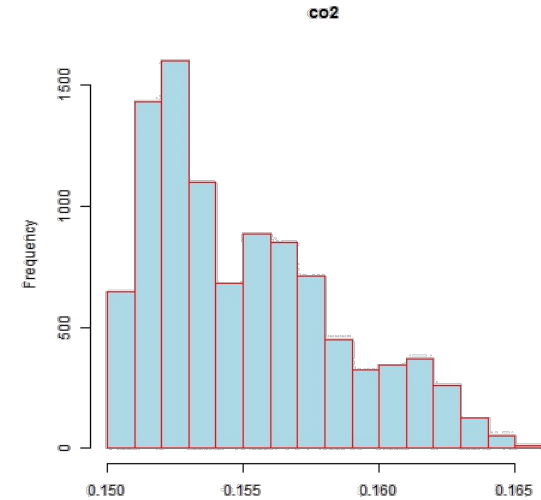
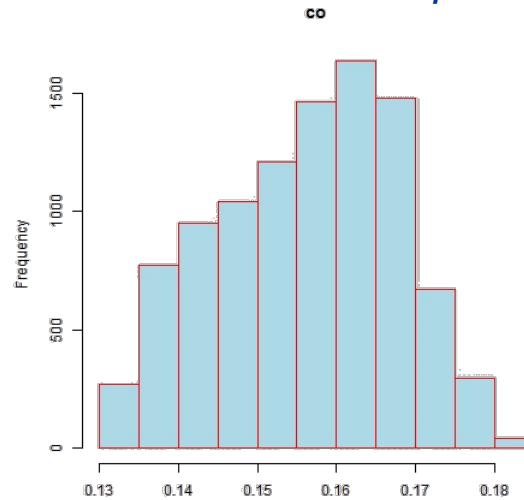
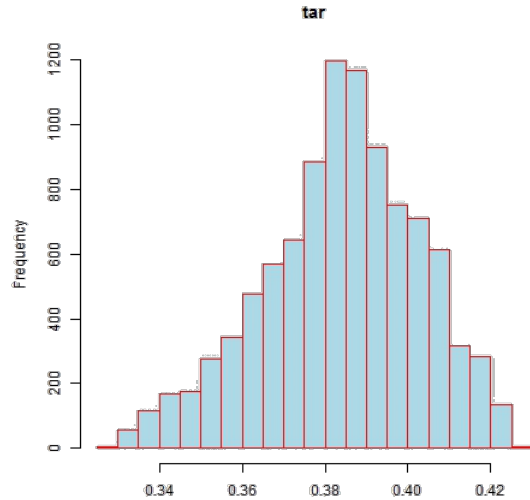
co [adjusted R² = 0.99774]

$-0.14732 + 2.2382e-006 * x + 1.1241e-009 * x^2 - 1.1396e-013 * x^3 + 4.5706e-013 * x^4 + 5.9254e-012 * x^2 * y + 0.00051444 * y - 1.6355e-007 * y^2 - 2.5615e-011 * y^3$ —
'summary_for_r.txt' every 1::2 u 1:2:6 *



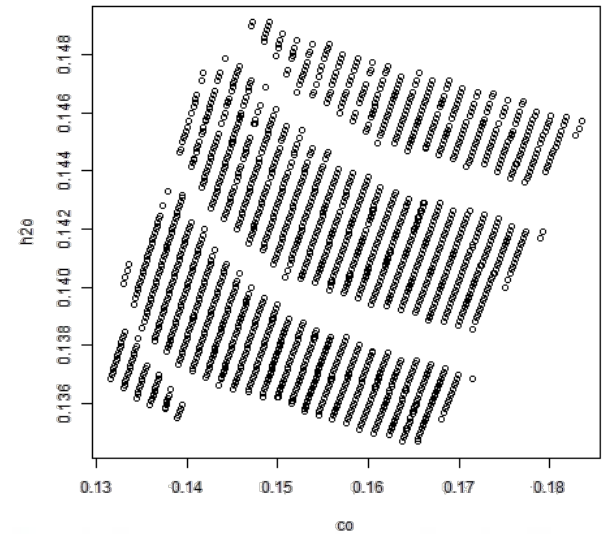
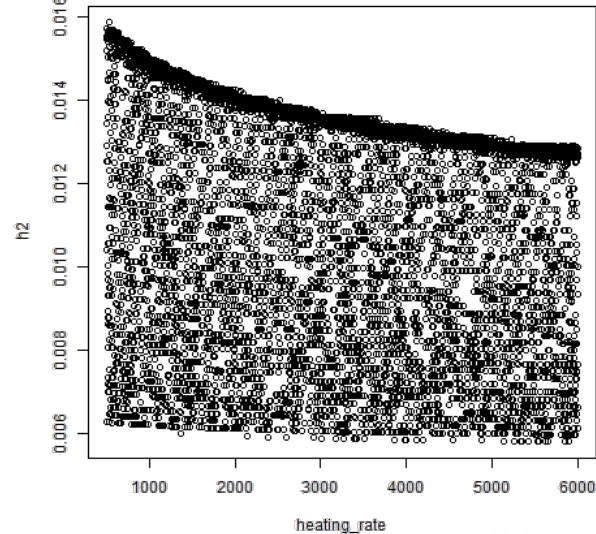
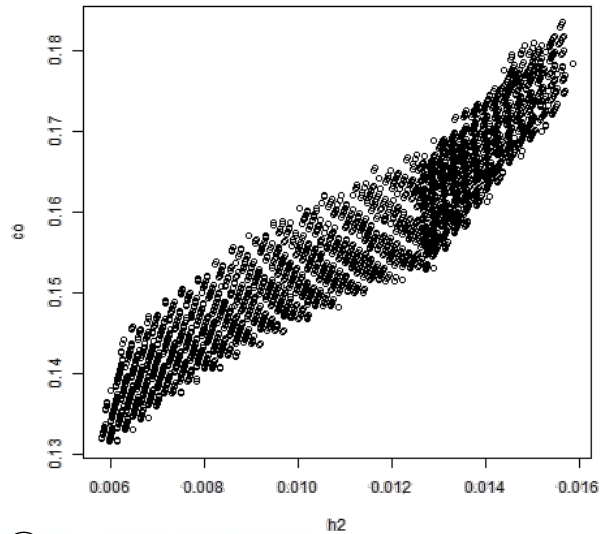
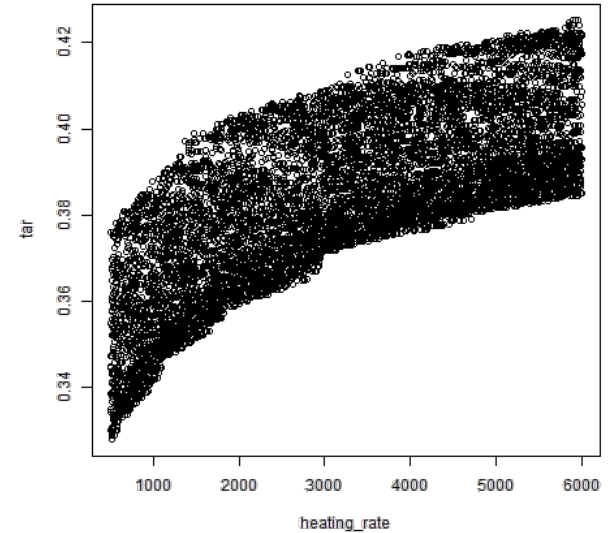
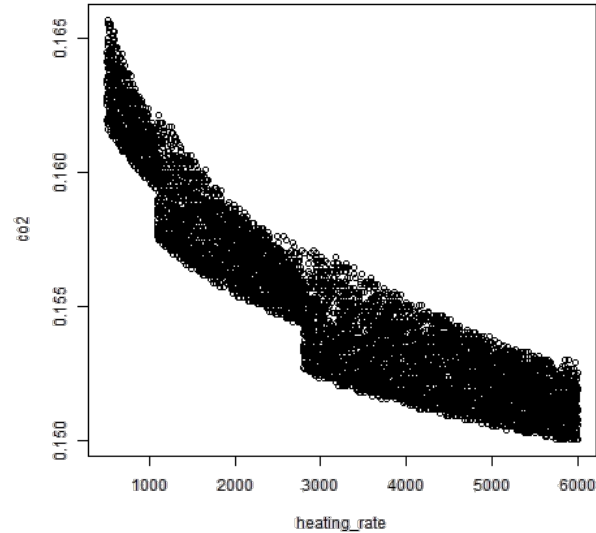
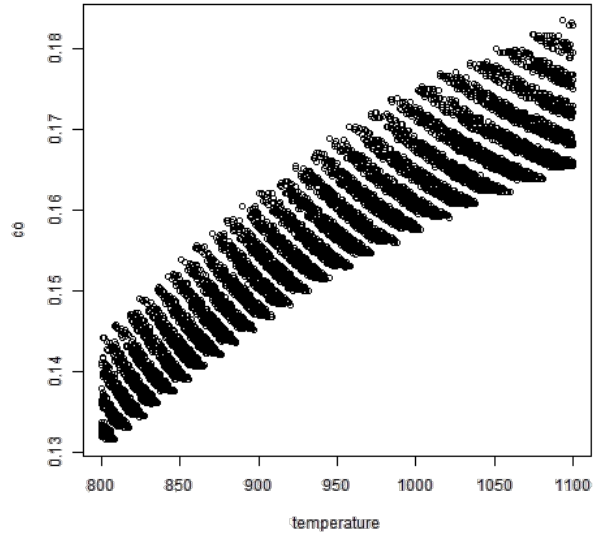
What's New in C3M?

*Uncertainty Quantification
PCCL with PRB Example*

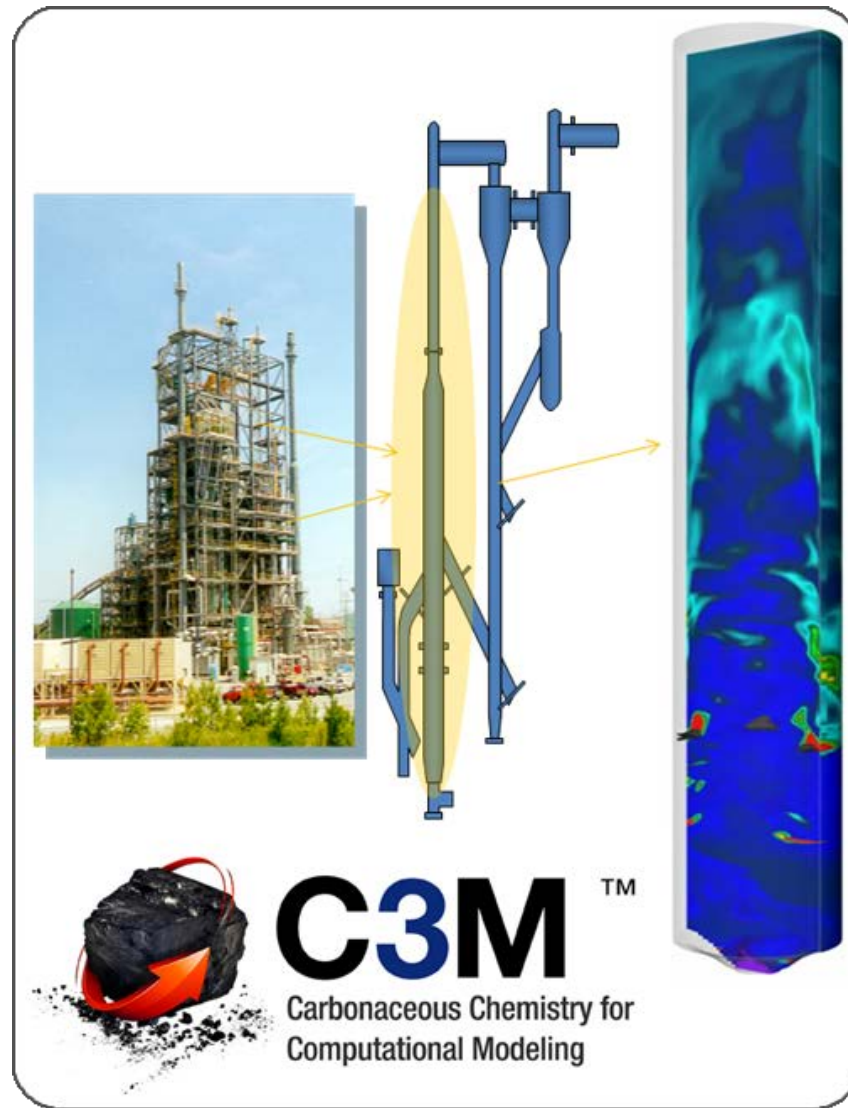


What's New in C3M?

*Uncertainty Quantification
PCCL with PRB Example*



Work Flow: Open C3M



Work Flow: Input Standard Fuel Properties

C:/C3M_Working_Dir/Project/ - C3M v. 2.0

File Tools Help

?

×

Add Fuel

Requirements

Proximate Analysis == 100
Ultimate Analysis == 100

Name: Illinois #6

Proximate Analysis

Fixed Carbon	Volatile Matter	Ash	Moisture
45.97	34.70	9.10	10.23

Normalize PA = 100

Ultimate Analysis - Dust Ash Free

Carbon	Hydrogen	Oxygen	Nitrogen	Sulfur
79.67	5.33	10.04	1.49	3.47

Normalize UA = 100

Summation

Proximate Analysis = 100
Ultimate Analysis = 100

Consistent PA

Consistent UA

Set

Cancel

Add

Remove

NATIONAL ENERGY TECHNOLOGY LABORATORY

Work Flow: Run All Desired Sub-Models

C:/C3M_Working_Dir/Project/ - C3M v. 2.0

File Tools Help

Illinois #6

Fuel

Proximate Analysis

Fixed Carbon	Volatile Matter	Ash	Moisture
45.97	34.70	9.10	10.23

Ultimate Analysis

Carbon	Hydrogen	Oxygen	Nitrogen	Sulfur
79.67	5.33	10.04	1.49	3.47

Kinetics

Chemistry Sub-Model

- Pyrolysis
- Char Oxidation
- Soot Oxidation
- Moisture Release
- Gasification
- Water Gas Shift
- Gas Phase Combustion
- Tar Oxidation

Kinetic Packages - Pyrolysis

- MGAS
- POCL**
- CPD
- FG-DVC
- NETL Co-Pyrolysis Data

Condition

Run

Equations

Devolatilization Only:

Volatile Matter $\rightarrow \alpha d_{Tar} + \beta d_{CO}CO + \beta d_{CO_2}CO_2 + \beta d_{CH_4}CH_4 + \beta d_{H_2}H_2 + \beta d_{H_2O}H_2O$
 $+ \beta d_{HCN}HCN + \beta d_{H_2S}H_2S + \beta d_{NH_3}NH_3 + \beta d_{C_2H_4}C_2H_4 + \beta d_{C_2H_6}C_2H_6 + \beta d_{C_3H_6}C_3H_6$
 $+ \beta d_{C_3H_8}C_3H_8$

$r_d = A \cdot \exp(-E_a / RT_s) \cdot \epsilon_s \cdot \rho_s \cdot (X_{vm} - X^*)$

$n_y = \beta d_y \cdot MW_{vm} / MW_y$

$y = VM, Tar, CO, CO_2, CH_4, H_2, H_2O, H_2S, NH_3, C_2H_2, C_2H_6, C_3H_6, C_6H_6; \beta d_{vm} = 1; \beta d_{Tar} = \alpha d$

$\beta d_i = MF_i / 100 \cdot (1 - FC_m)$

$\alpha d = 1 - \sum_i \beta d_i$

$X^* = (X_{vm}^0 + X_{FC}^0) \cdot X_{min}^*$

Add Remove

Work Flow: Run All Desired Sub-Models

C:/C3M_Working_Dir/Project/ - C3M v. 2.0

File Tools Help

Illinois #6

Fuel

Proximate Analysis

Fixed Carbon	Volatile Matter	Ash	Moisture
45.97	34.70	9.10	10.23

Ultimate Analysis

Carbon	Hydrogen	Oxygen	Nitrogen	Sulfur
79.67	5.33	10.04	1.49	3.47

Kinetics

Chemistry Sub-Model

Pyrolysis
Char Oxidation
Soot Oxidation
Moisture
Gasification
Water Gas
Gas Phase
Tar Oxidation

Kinetic Packages - Pyrolysis

MGAS
PCCL
CPD

Condition

PCCL Testplan Data

☐ Not Specified
☐ Sweep TGAS
☐ Sweep Pressure
☐ Sweep DP
☒ Sweep Heating Rate

☒ Devolatilization Only
☐ Tar Cracking
☐ Secondary Pyrolysis/
Soot Formation

Set Cancel

Equation

Devolatilization Only:

Volatile Matter $\rightarrow \alpha d_{Tar} + \beta d_{CO}CO + \beta d_{CO_2}CO_2 + \beta d_{CH_4}CH_4 + \beta d_{H_2}H_2 + \beta d_{H_2O}H_2O$
 $+ \beta d_{HCN}HCN + \beta d_{H_2S}H_2S + \beta d_{NH_3}NH_3 + \beta d_{C_2H_4}C_2H_4 + \beta d_{C_2H_6}C_2H_6 + \beta d_{C_3H_6}C_3H_6$
 $+ \beta d_{C_3H_8}C_3H_8$

$r_d = A \cdot \exp(-E_a / RT_s) \cdot \epsilon_s \cdot \rho_s \cdot (X_{VM} - X^*)$

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$\beta d_i = MF_i / 100 \cdot (1 - FC_m)$

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Add Remove

Work Flow: Run All Desired Sub-Models

C:/C3M_Working_Dir/Project/ - C3M v. 2.0

File Tools Help

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Kinetics

Chemistry Sub-Model

Pyrolysis
Char Oxidation
Soot Oxidation
Moisture
Gasification
Water Gas
Gas Phase
Tar Oxidation

Kinetic Packages - Pyrolysis

MGAS
PCCL
CPD

Condition

PCCL Testplan Data

Condition

Condition Name
Heating Rate = 500

OK Cancel

Set Cancel

Equation

Devolatilization Only:

Volatile Matter $\rightarrow \alpha d_{Tar} + \beta d_{CO}CO + \beta d_{CO_2}CO_2 + \beta d_{CH_4}CH_4 + \beta d_{H_2}H_2 + \beta d_{H_2O}H_2O$
 $+ \beta d_{HCN}HCN + \beta d_{H_2S}H_2S + \beta d_{NH_3}NH_3 + \beta d_{C_2H_4}C_2H_4 + \beta d_{C_2H_6}C_2H_6 + \beta d_{C_3H_6}C_3H_6$
 $+ \beta d_{C_3H_8}C_3H_8$

$r_d = A \cdot \exp(-E_a / RT_s) \cdot \epsilon_s \cdot \rho_s \cdot (X_{VM} - X^*)$

$n_y = \beta d_y \cdot MW_{VM} / MW_y$

$y = VM, Tar, CO, CO_2, CH_4, H_2, H_2O, H_2S, NH_3, C_2H_2, C_2H_6, C_3H_6, C_6H_6; \beta d_{VM} = 1; \beta d_{Tar} = \alpha d$

$\beta d_i = MF_i / 100 \cdot (1 - FC_m)$

$\alpha d = 1 - \sum_i \beta d_i$

$X^* = (X_{VM}^0 + X_{FC}^0) \cdot X_{min}^*$

Add Remove

Work Flow: Run All Desired Sub-Models

C:\C3M_Working_Dir\Project\ - C3M v. 2.0

File Edit View Help PC Coal Lab File Setup

Fuel Description

COAL_NAME

FC	PVM	Ash	Moisture
45.97	34.7	9.1	10.23

coal # 1

%C	%H	%O	%N	%S
79.67	5.33	10.04	1.49	3.47

Write to Coalpc execute read a Coalpc.dat file Get Properties from DB

label by Operating conditions Rate law Calculate rate parameters for... Report options

TI ☐ Tinitial (C) 25 ☒ SFDR ☒ Weight loss ☒ Major products

TG ☐ T(ultimate (C)) 1226.85 ☐ DAEM ☒ Tar release ☒ Noncondensable gases

Q, (C/s) 500 ☐ C2SM ☒ Gas release ☒ Hydrocarbons

O2 ☐ %O2 0 ☒ CO2 release ☒ Nitrogen-species

PT ☐ P (MPa) 0.506625 ☒ H2O release ☒ Oxygen-species

TR/QQ ☒ T[tp] (s) 4 ☒ CO release ☒ Tar compositions

DP ☐ dp (micron) 100 ☒ Hydrocarbon release ☒ Char compositions

☐ HCN release ☒ Assign global devolatilization rates

☐ Volatile-nitrogen release Report secondary pyrolysis products

☐ Char-nitrogen evolution ☐ Y ☐ N ☐ T

☒ Assign global char conversion rates

☒ Report char conversion histories

Test Sequence ☐ FF ☒ Sw

show screen output

Write to Testplan

condition # 1

read a testplan.dat file

☐ drop tube ☒ wire grid

Work Flow: Run All Desired Sub-Models

C:/C3M_Working_Dir/Project/ - C3M v. 2.0

File Tools Help

Illinois #6

Fuel

Proximate Analysis

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- Tar Oxidation

Kinetic Packages - Pyrolysis

- MGAS
- PCCL
- CPD
- FG-DVC
- NETL Co-Pyrolysis Data

Condition

- Heating Rate = 500
- Heating Rate = 1000
- Heating Rate = 1500

Run

Equations

Devolatilization Only:

Volatile Matter \rightarrow $0.497133 + 0.086218\text{CO} + 0.0452645\text{CO}_2 + 0.0775962\text{CH}_4 + 0.0310385\text{H}_2 + 0.112083\text{H}_2\text{O} + 0.0125016\text{HCN} + 0.0676812\text{H}_2\text{S} + 0\text{NH}_3 + 0.0334095\text{C}_2\text{H}_4 + 0.00991507\text{C}_2\text{H}_6 + 0.0271587\text{C}_3\text{H}_6 + 0\text{C}_3\text{H}_8$

$r_d = 107.9 * \exp(-7060 / RT_s) * \epsilon_s * \rho_s * (X_{vm} - X^*)$

$n_y = \beta_{d_y} * MW_{vm} / MW_y$

$y = \text{VM, Tar, CO, CO}_2, \text{CH}_4, \text{H}_2, \text{H}_2\text{O, H}_2\text{S, NH}_3, \text{C}_2\text{H}_2, \text{C}_2\text{H}_6, \text{C}_3\text{H}_6, \text{C}_6\text{H}_6; \beta_{d_{vm}} = 1; \beta_{d_{tar}} = \alpha d$

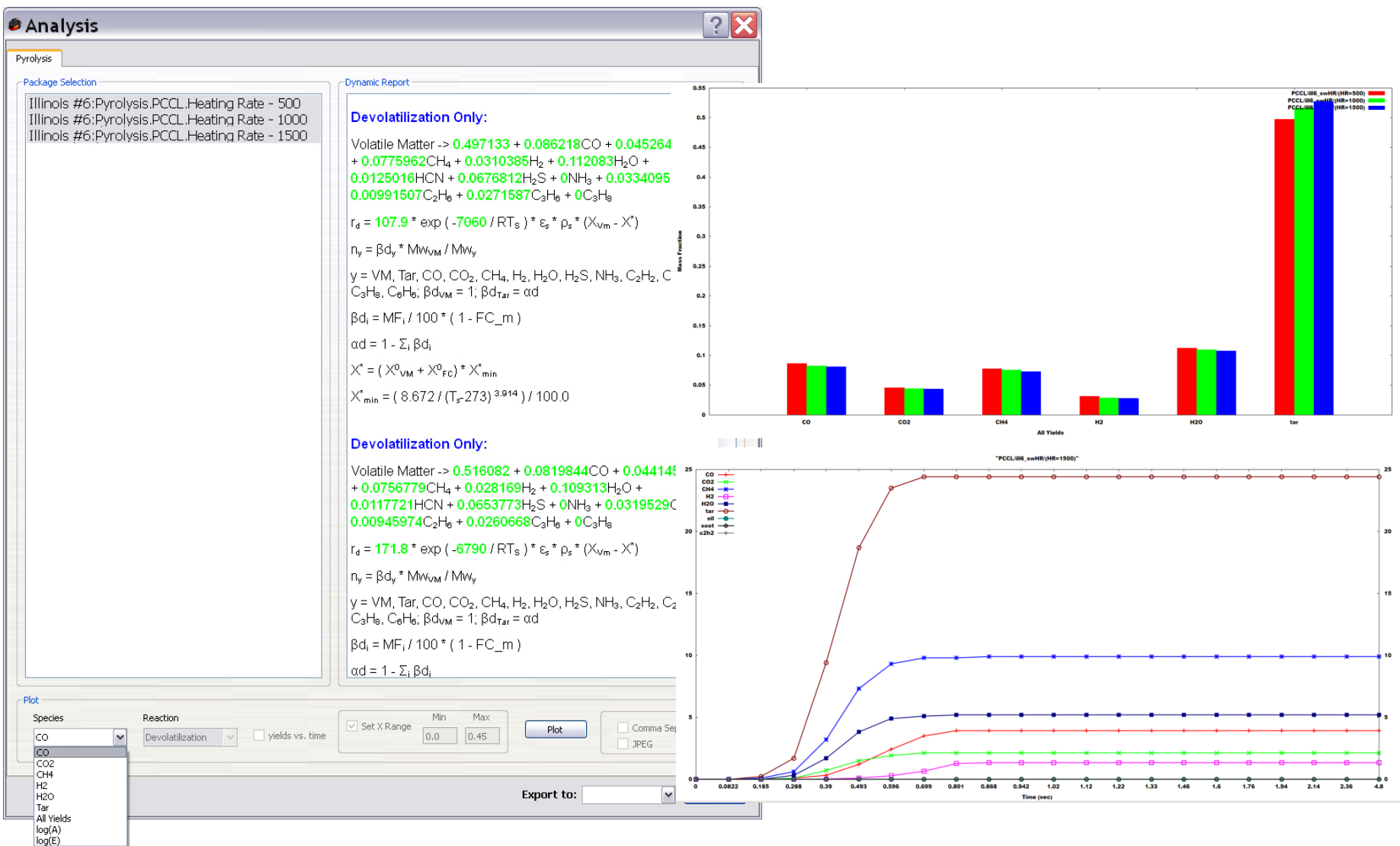
$\beta_{d_i} = MF_i / 100 * (1 - FC_m)$

$\alpha d = 1 - \sum \beta_{d_i}$

$X^* = (X_{vm}^0 + X_{fc}^0) * X_{min}^*$

Add Remove

Work Flow: Compare Results



Work Flow: Select Input for Global Model

Export

Illinois #6

Kinetics

Pyrolysis
Gasification
Water Gas Shift
Condensed Phase Combustion
Gas Phase Combustion
Tar Combustion

MGAS
PCCL
CPD
FG-DVC
NETL Co-Pyrolysis Data

☒ Heating Rate = 500
☐ Heating Rate = 1000
☐ Heating Rate = 1500

Dynamic Report

Devolatilization Only:

Volatile Matter -> 0.497133 + 0.086218CO + 0.0452645CO₂ + 0.0775962CH₄ +
0.0310385H₂ + 0.112083H₂O + 0.0125016HCN + 0.0676812H₂S + 0NH₃ +
0.0334095C₂H₄ + 0.00991507C₂H₆ + 0.0271587C₃H₈ + 0C₃H₆

$r_d = 107.9 * \exp(-7060 / RT_s) * \epsilon_s * \rho_s * (X_{vm} - X^*)$

$n_y = \beta_{d_y} * M_{w_{vm}} / M_{w_y}$

$y = VM, Tar, CO, CO_2, CH_4, H_2, H_2O, H_2S, NH_3, C_2H_2, C_2H_6, C_3H_8, C_6H_6; \beta_{d_{vm}} = 1; \beta_{d_{Tar}} = \alpha_d$

$\beta_{d_i} = MF_i / 100 * (1 - FC_m)$

Add Remove

CFD Code:

▼

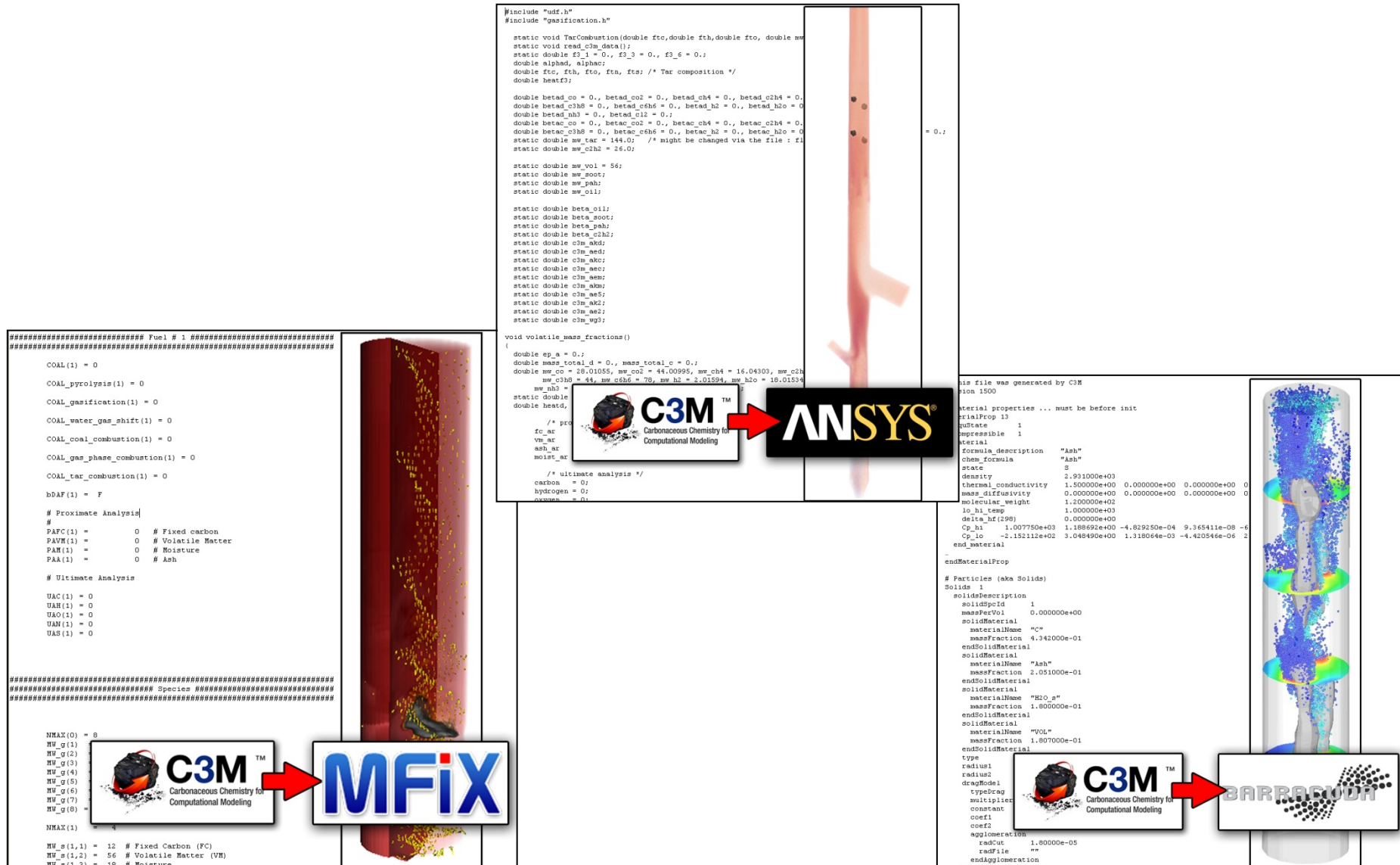
MFiX
ANSYS FLUENT
BARRACUDA
Report

Export

<#>

NATIONAL ENERGY TECHNOLOGY LABORATORY

Work Flow: Generate Input Files for CFD



The Future of C3M

Uncertainty Quantification

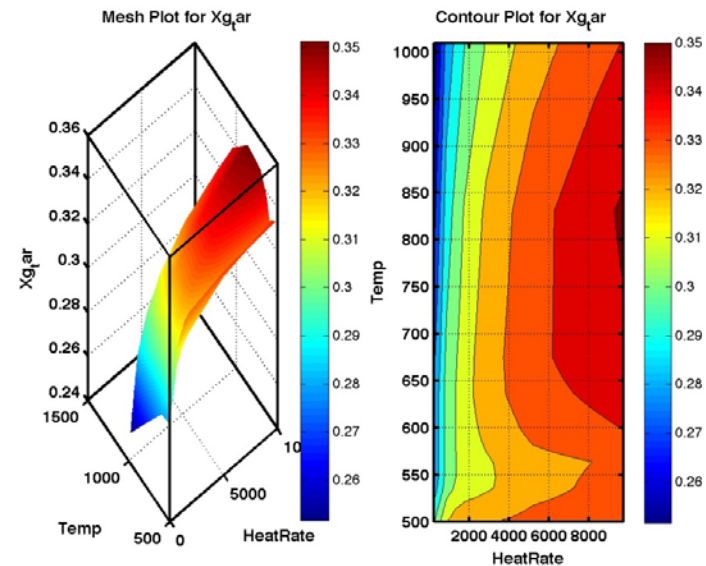
- **In order to accelerate technology deployment from pilot scale to commercial scale, CFD model predictions have to take into account and quantify various sources of uncertainty.**
 - Identify and characterize all sources of uncertainty (Aleatory or Epistemic)
 - uncertainty due to numerical approximations (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 ($\mu = 3000$, $\sigma = 1000$)
 - Temperature: Normal ($\mu = 800$, $\sigma = 100$)
 - Pressure: Normal ($\mu = 2000$, $\sigma = 500$)
- **Propagation of input uncertainties are examined by 10,000 Direct MC simulation and 10,000 MC simulation via surrogate model**

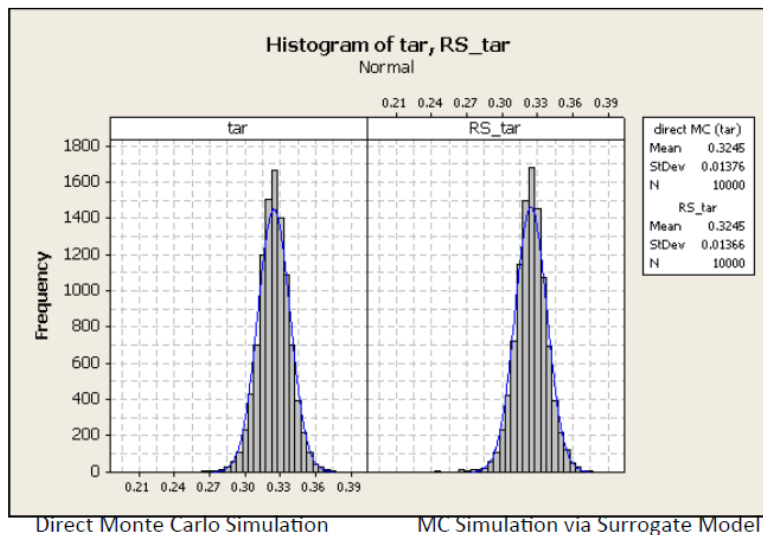


Response surface for propagating input uncertainty in tar pyrolysis process

The Future of C3M

Uncertainty Quantification

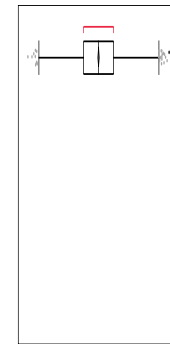
Example: Gas Production response to Heating Rate, Temp., and Press. within the PCCL pyrolysis model



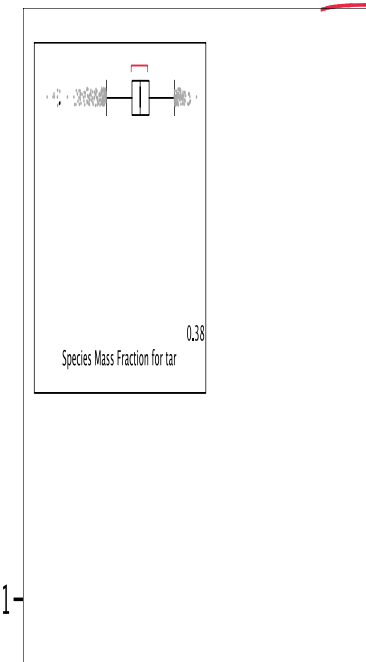
No major differences in the output parameters between direct MC simulation and MC simulation via surrogate model

0.1-

-



0.1-



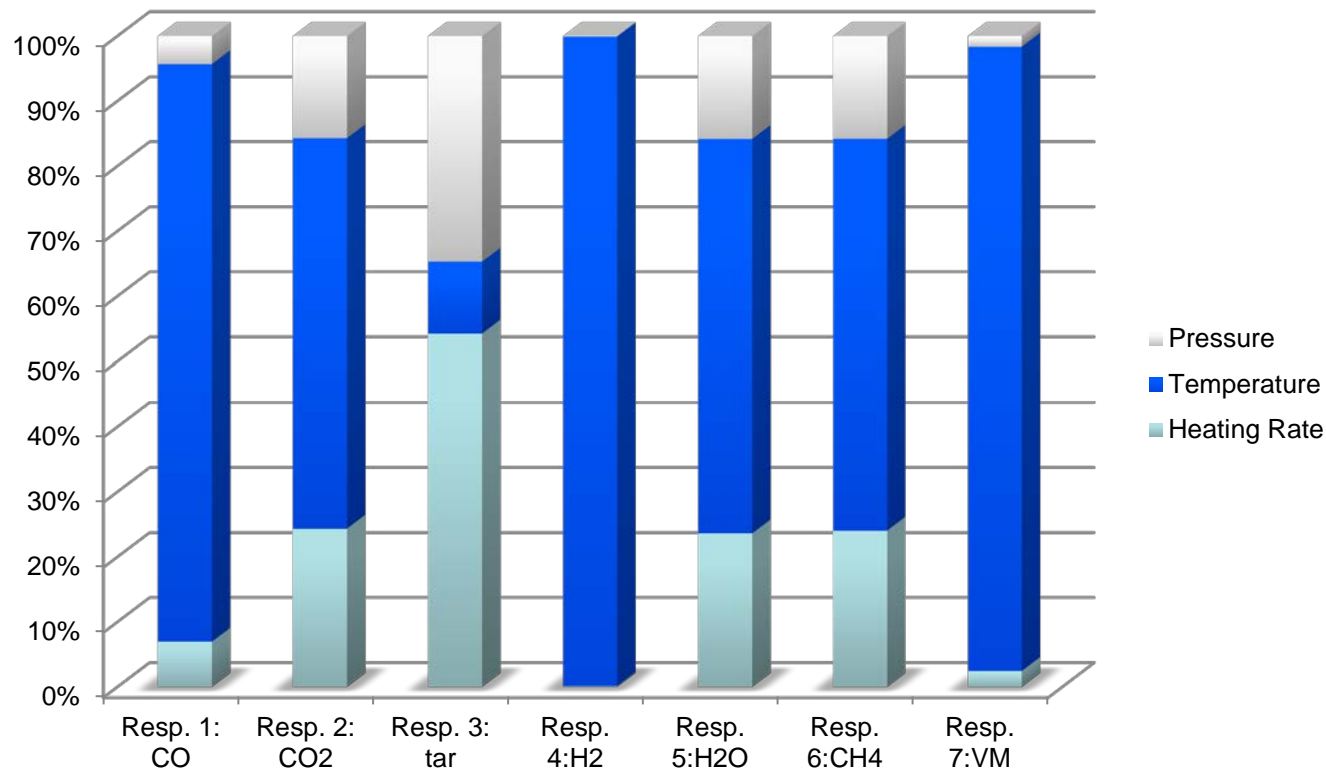
Cumulative Density Function plots generated via Direct Monte Carlo simulation to assess the likelihood of achieving desired level of species under prescribed input uncertainties

The Future of C3M

Uncertainty Quantification

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

Sensitivity of Gas Products to Input Variables



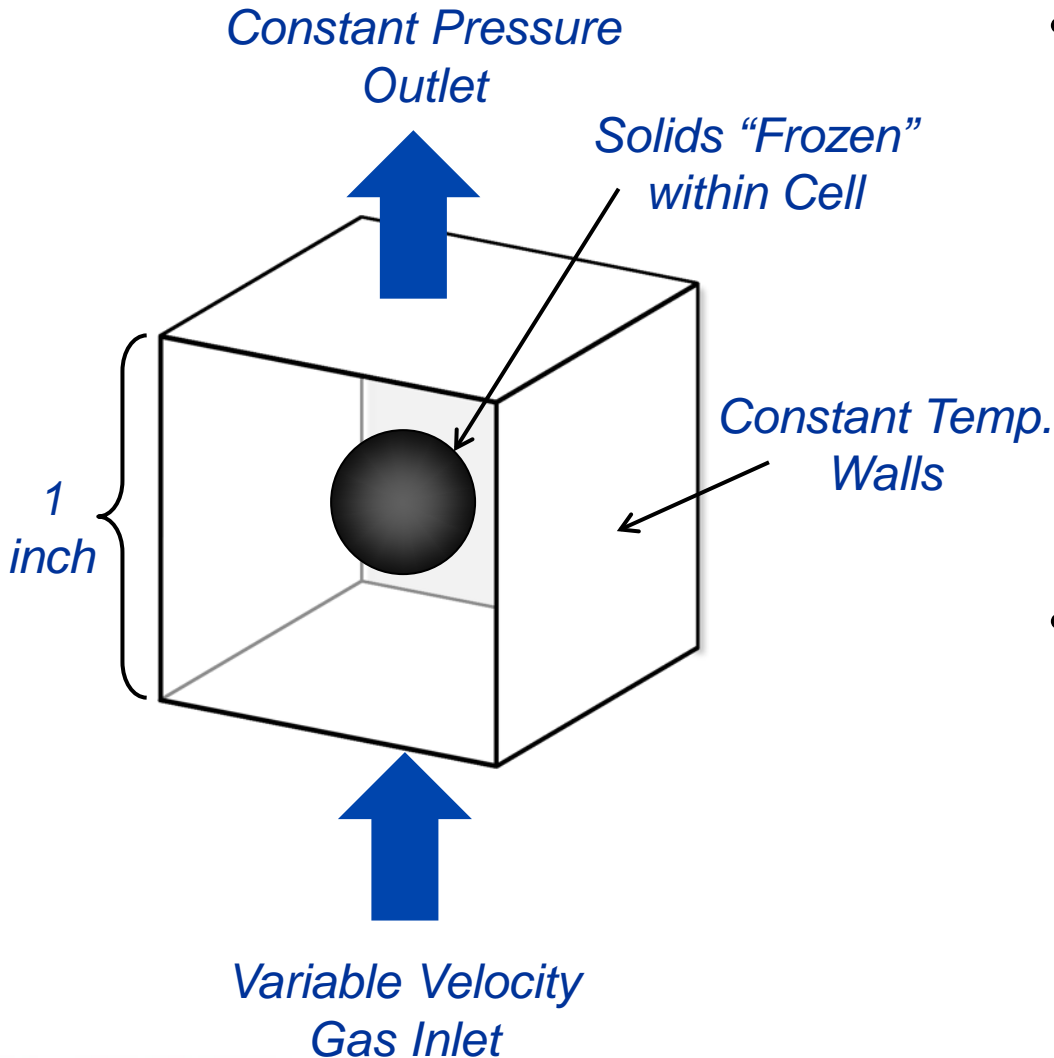
The Future of C3M

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**

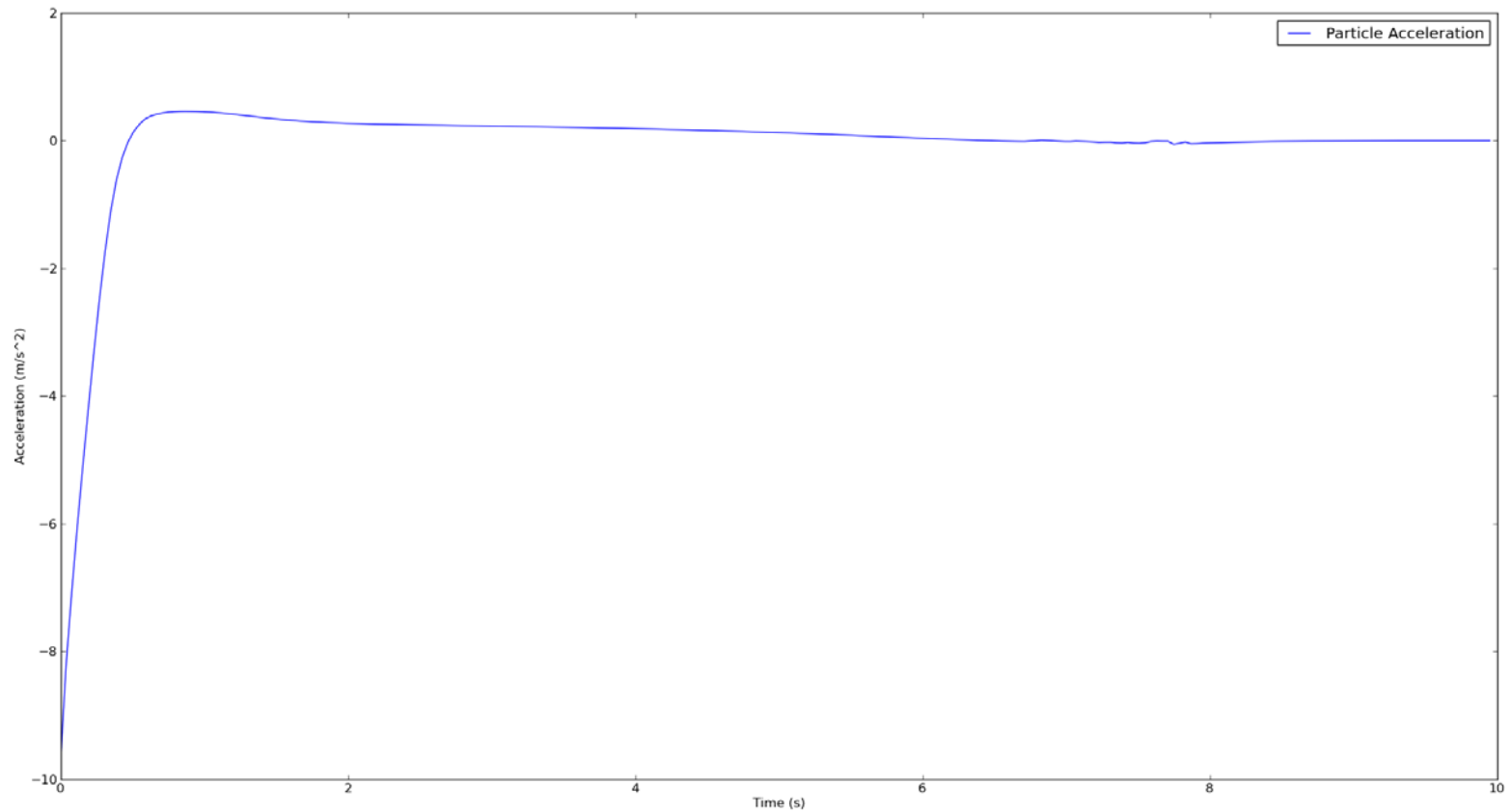
- $V_{\text{inlet_init}} = 0.01 \text{ m/s}$
- $T_{\text{gas_init}} = 1200 \text{ K}$
- $T_{\text{solid}} = 300 \text{ K}$
- $D_p = 200 \times 10^{-6} \text{ m}$
- $\theta_s = 0.001$
- $\rho_s = \text{Mixture Law}$
- $C_{s_init} = \text{Set By C3M}$
- $C_{g_init} = [\text{CO}=.05, \text{CO}_2=.05, \text{H}_2=.05, \text{O}_2=0.1, \text{H}_2\text{O}=0.75]$

- **Boundary Conditions**

- $P_{\text{outlet}} = 1 \text{ atm}$
- $T_{\text{wall}} = 1200 \text{ K}$
- $T_{\text{gas_inlet}} = 1200 \text{ K}$
- $V_{\text{gas_inlet}} = -\text{SFFV}$
- $C_{g_inlet} = C_{g_init}$

Work Flow: Analyze Results

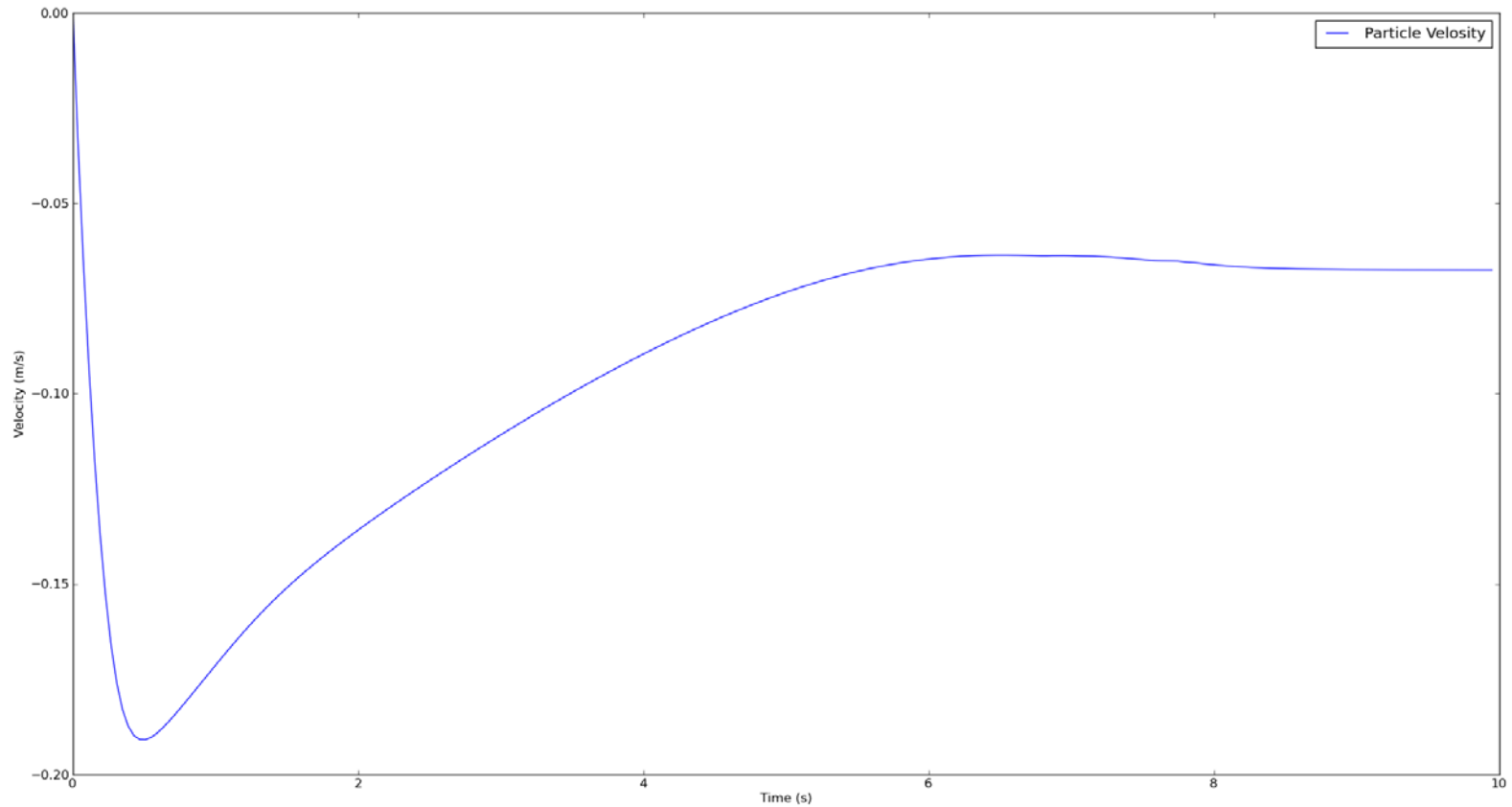
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



Result: Particle Acceleration

Work Flow: Setup and Run CFD

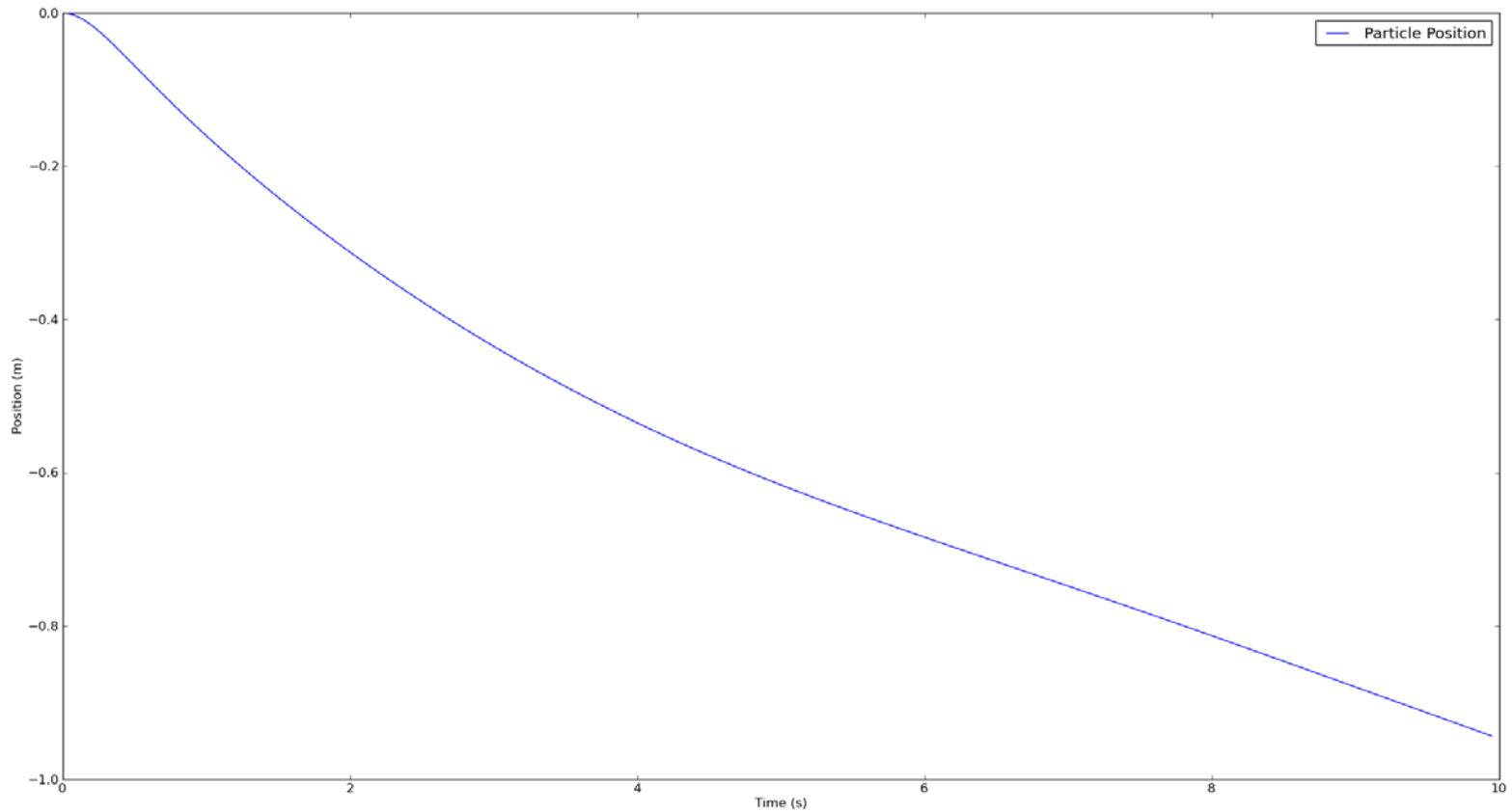
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



Result: Particle Velocity

Work Flow: Virtual Drop Tube

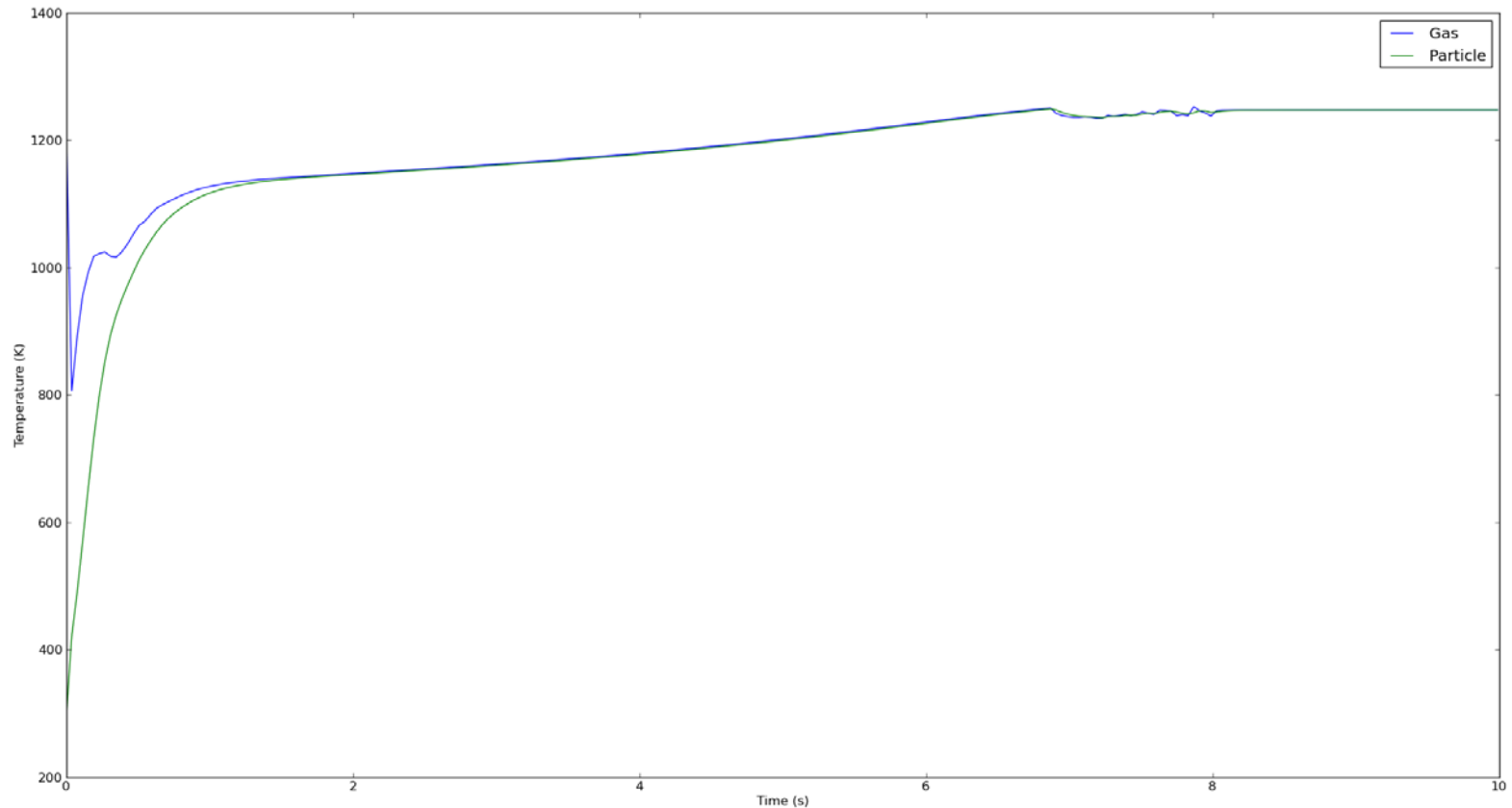
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



Result: Particle Position

Work Flow: Setup and Run CFD

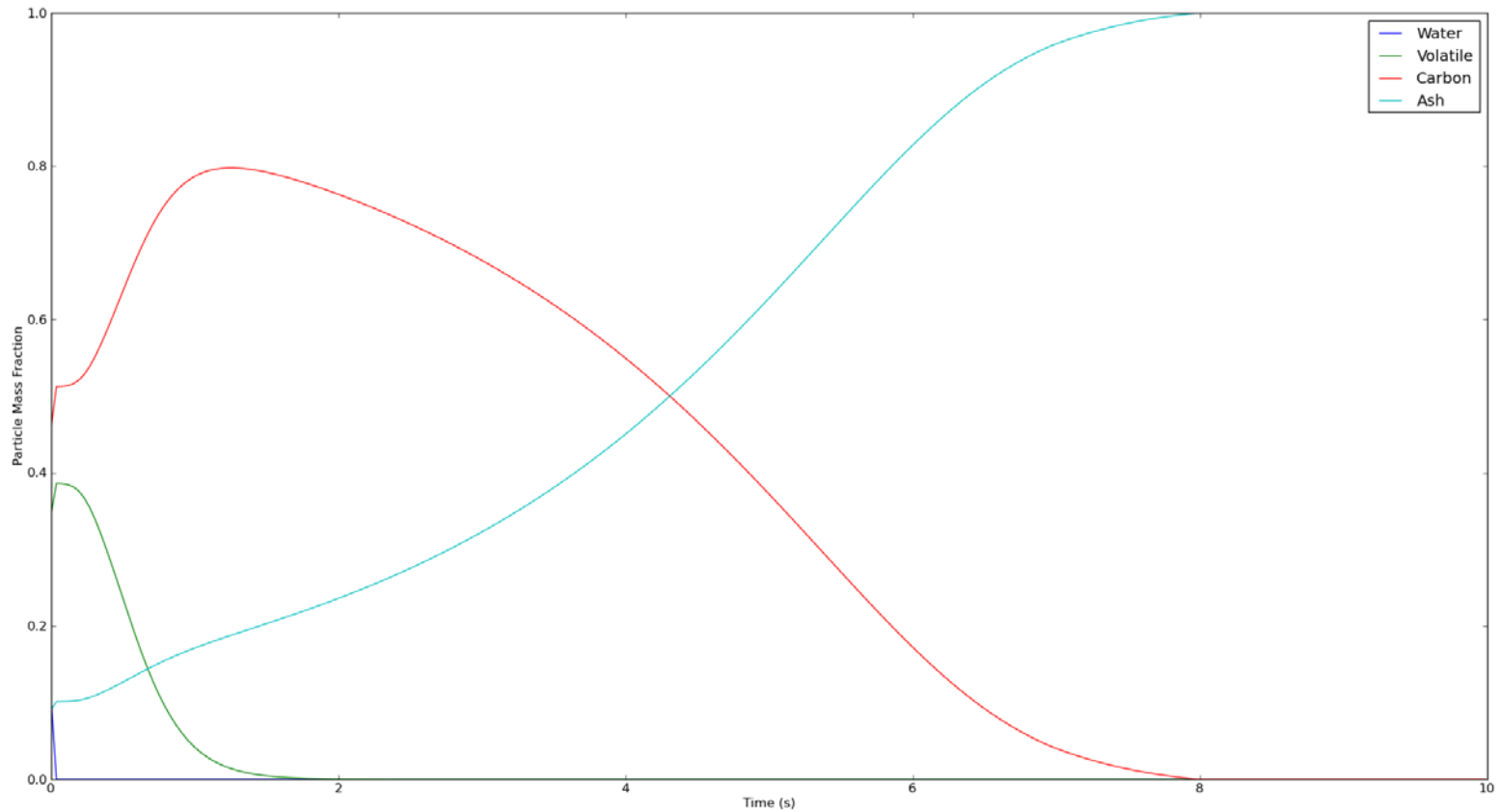
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



Result: Gas and Particle Temperature

Work Flow: Setup and Run CFD

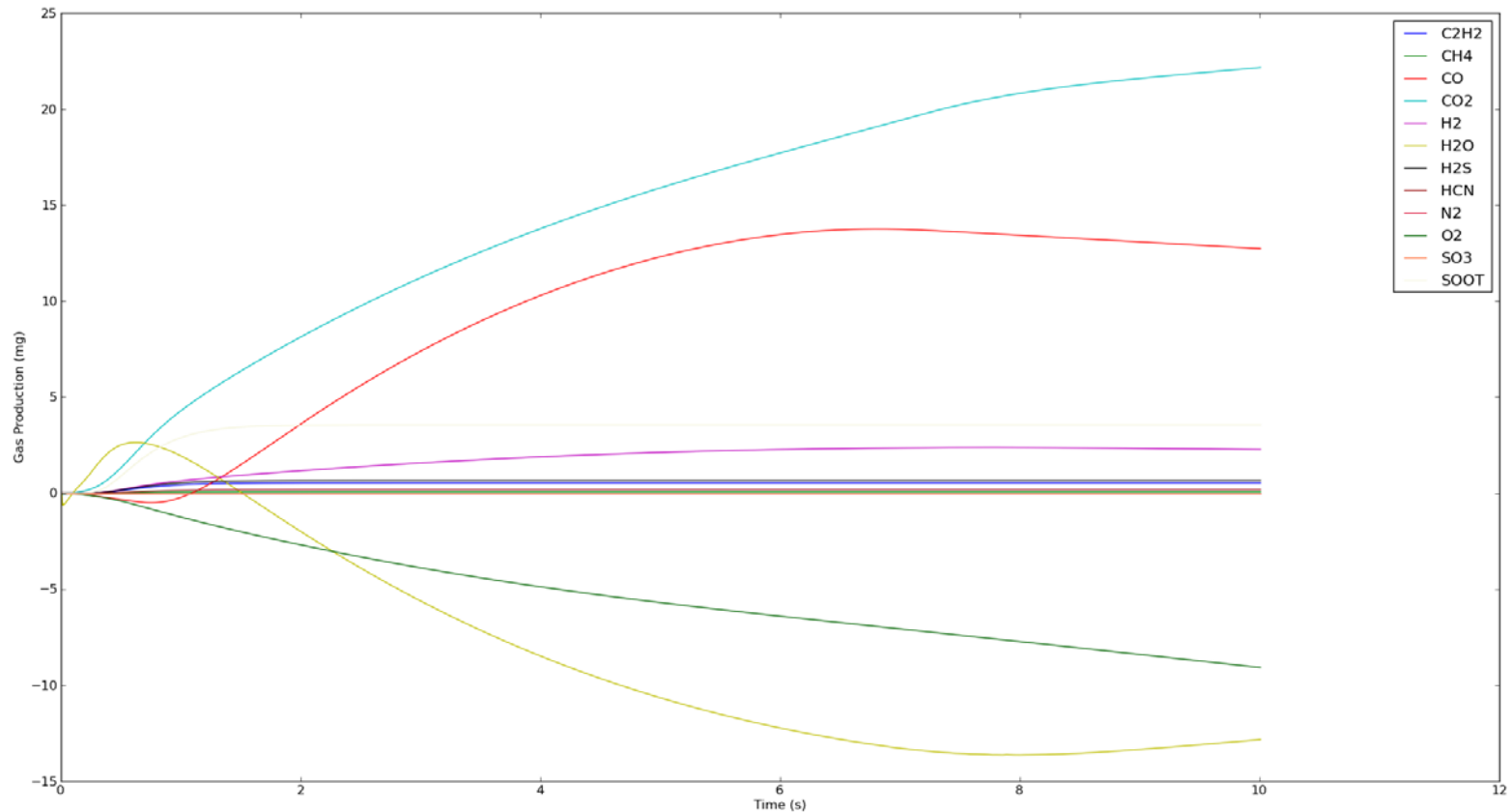
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



Result: Mass Fraction of Solid Species within Particle

Work Flow: Setup and Run CFD

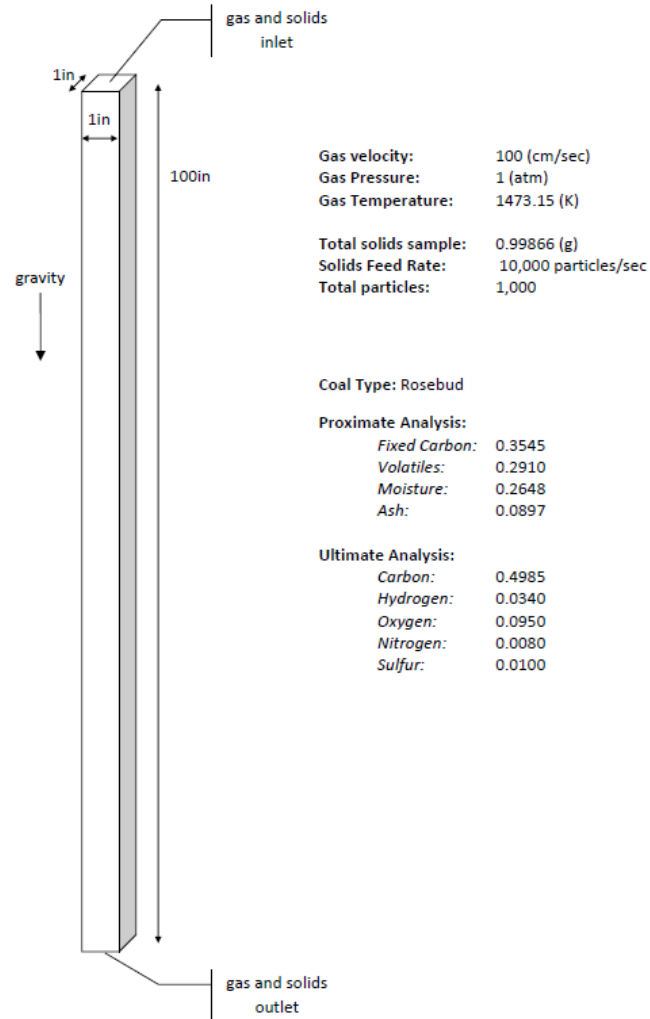
Example: Single Cell Virtual Drop Tube with Python Controller Running Barracuda Solver



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

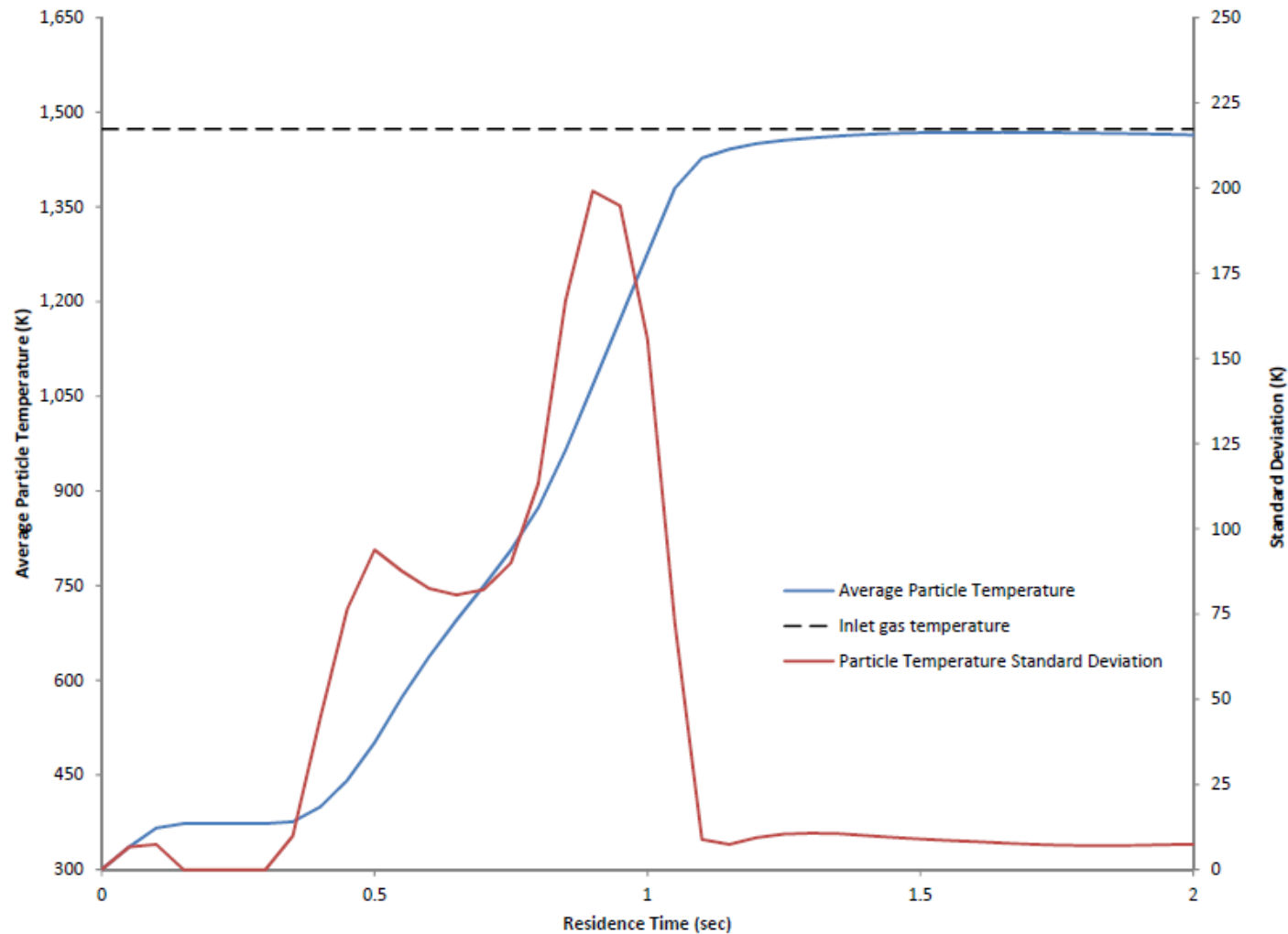
Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



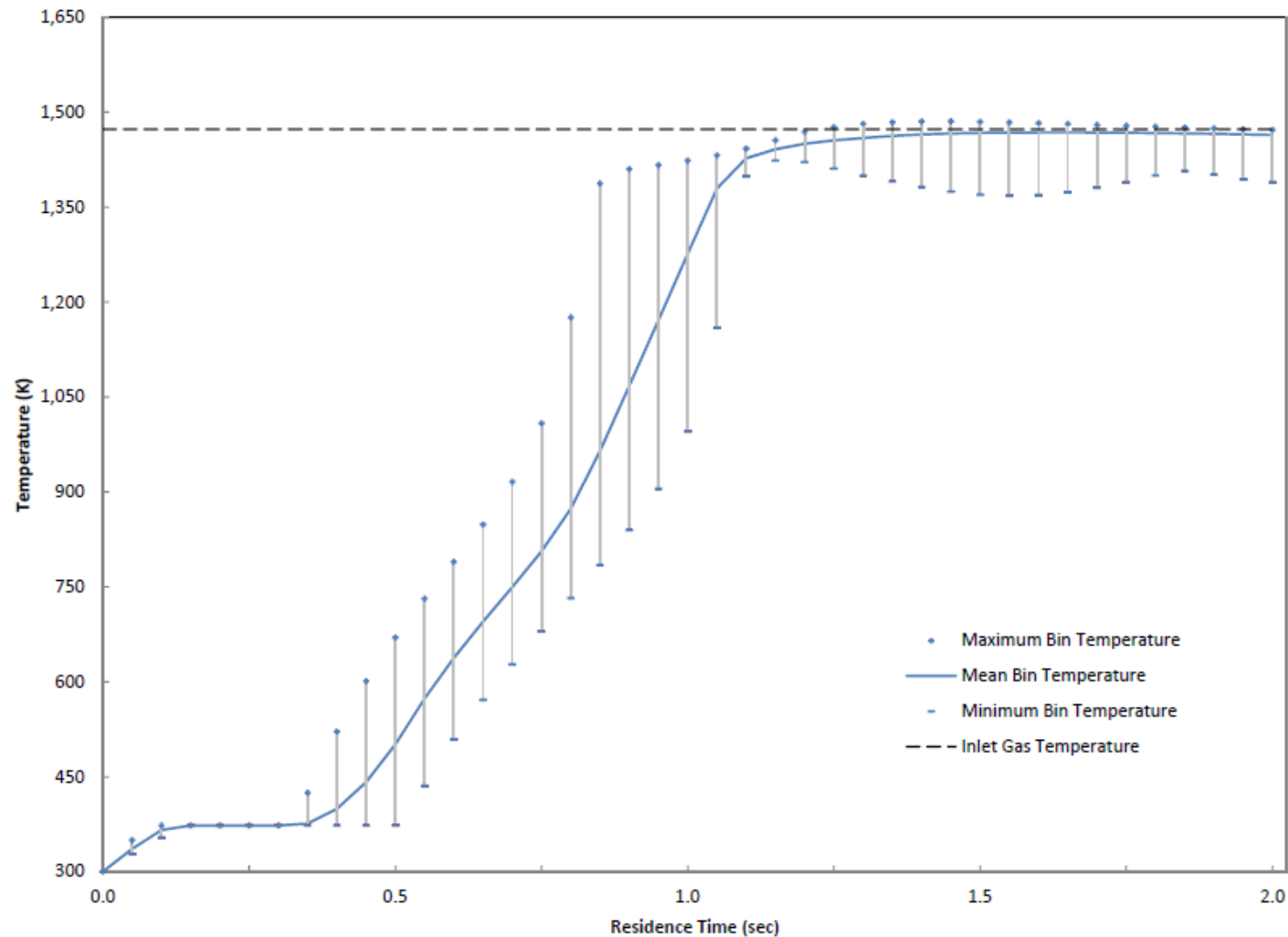
Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



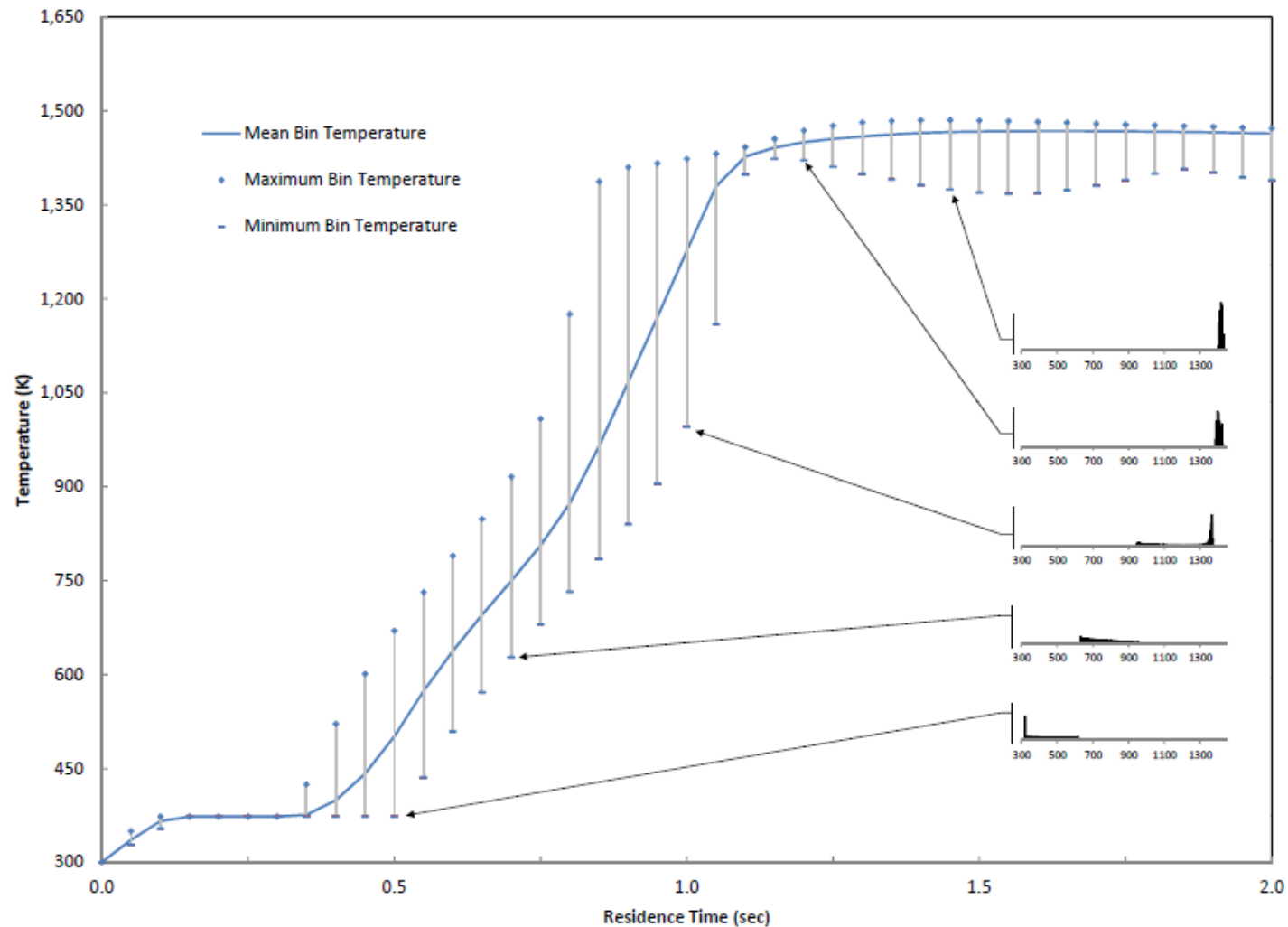
Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



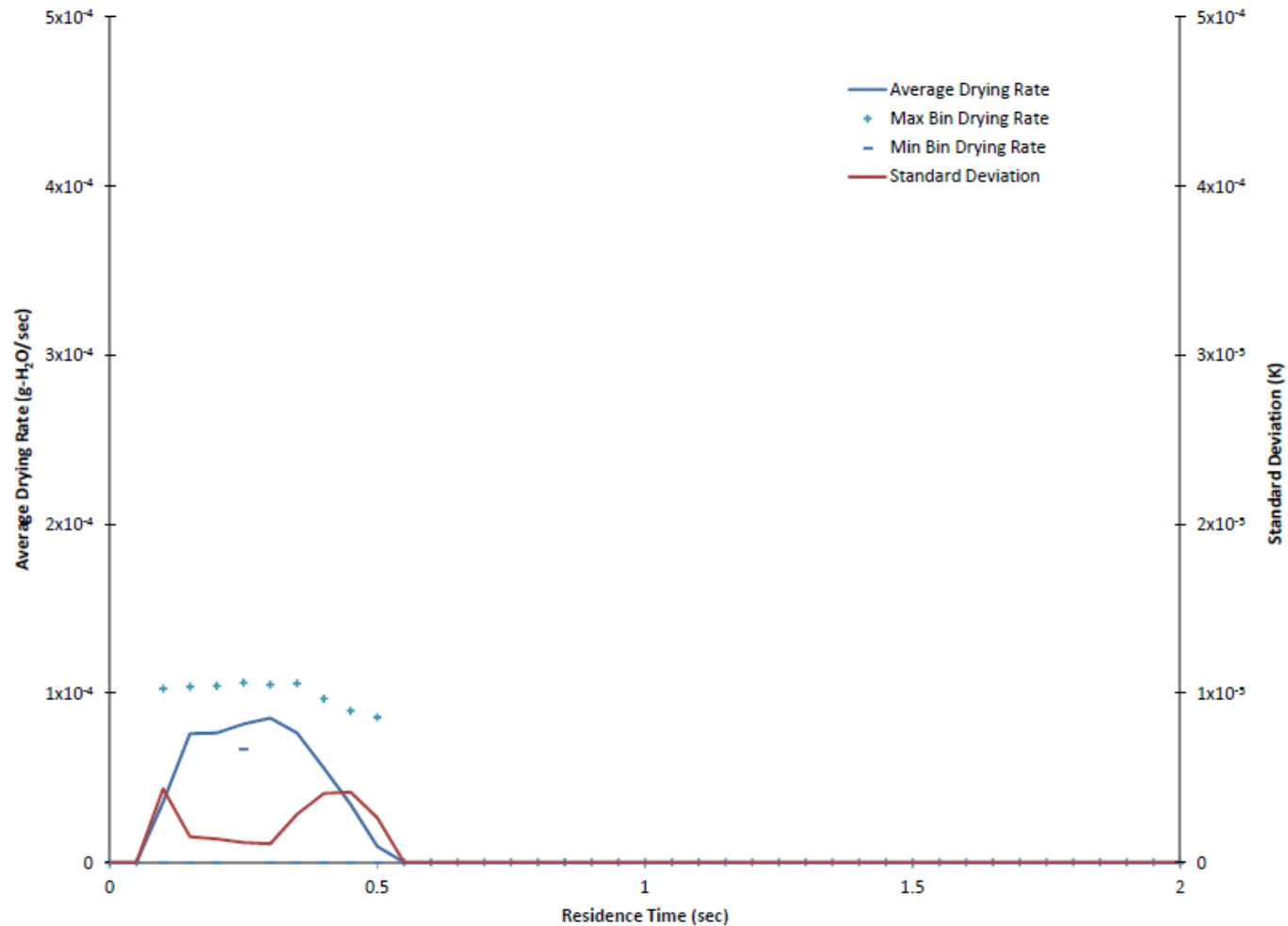
Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



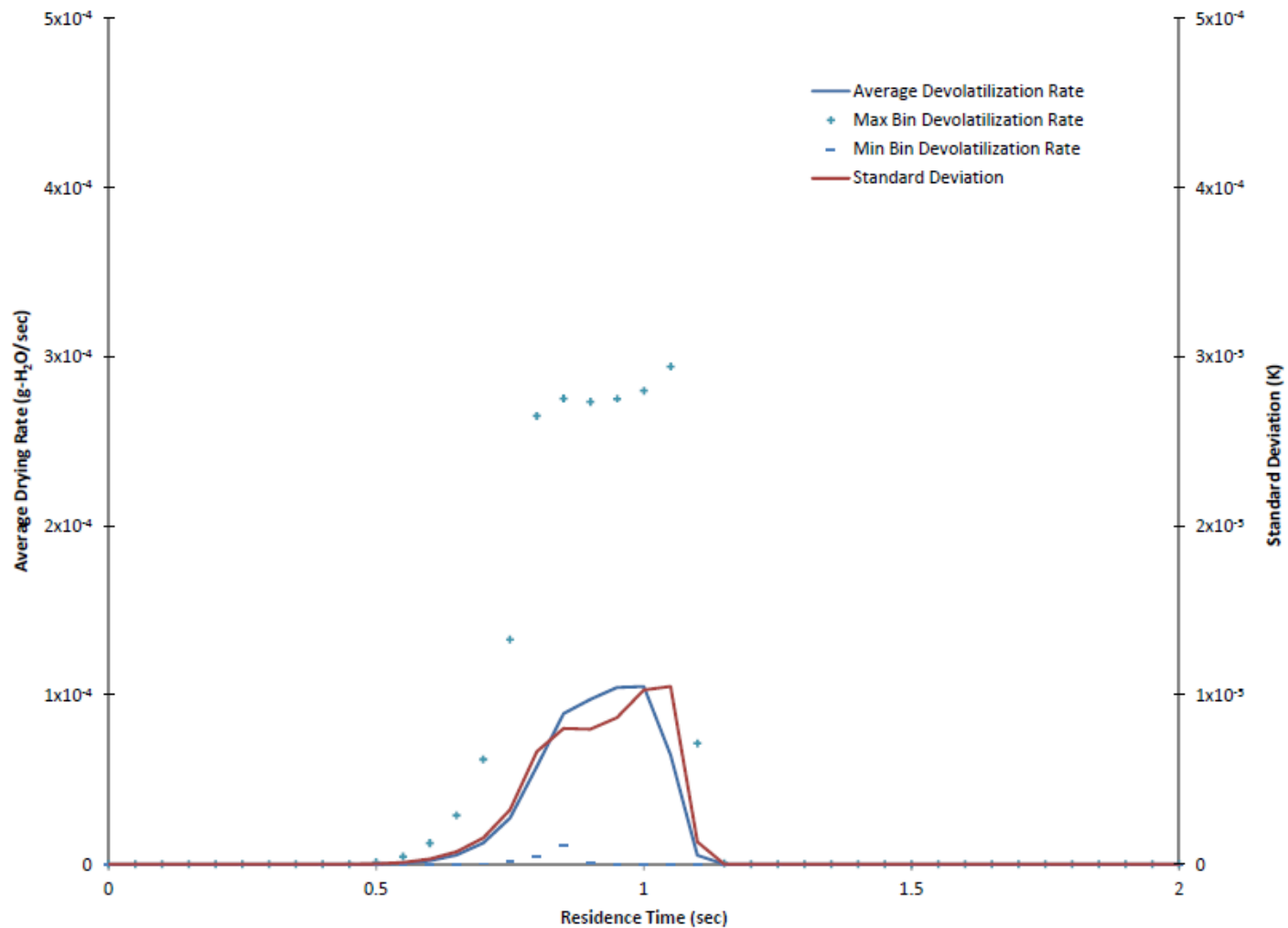
Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



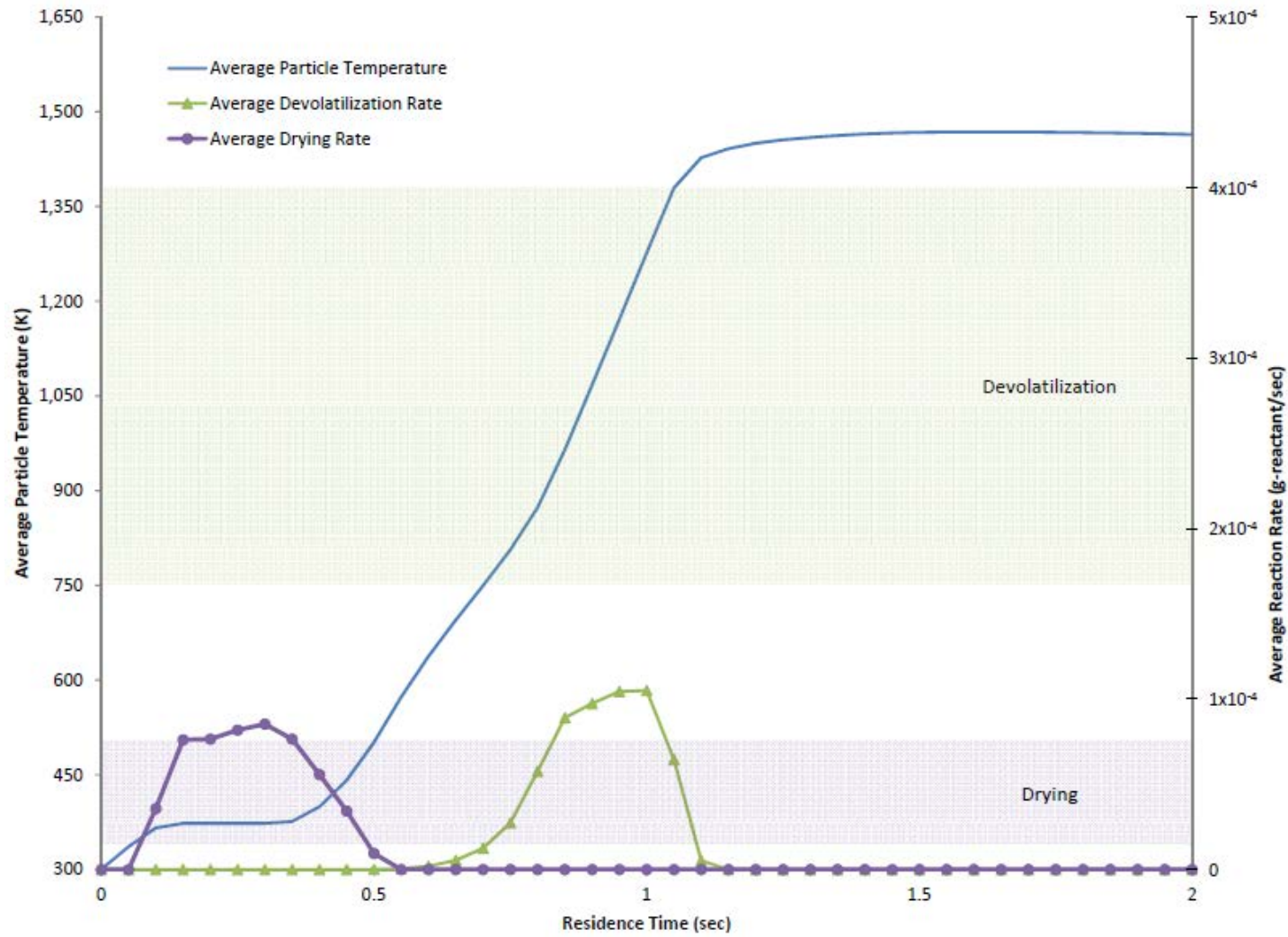
Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



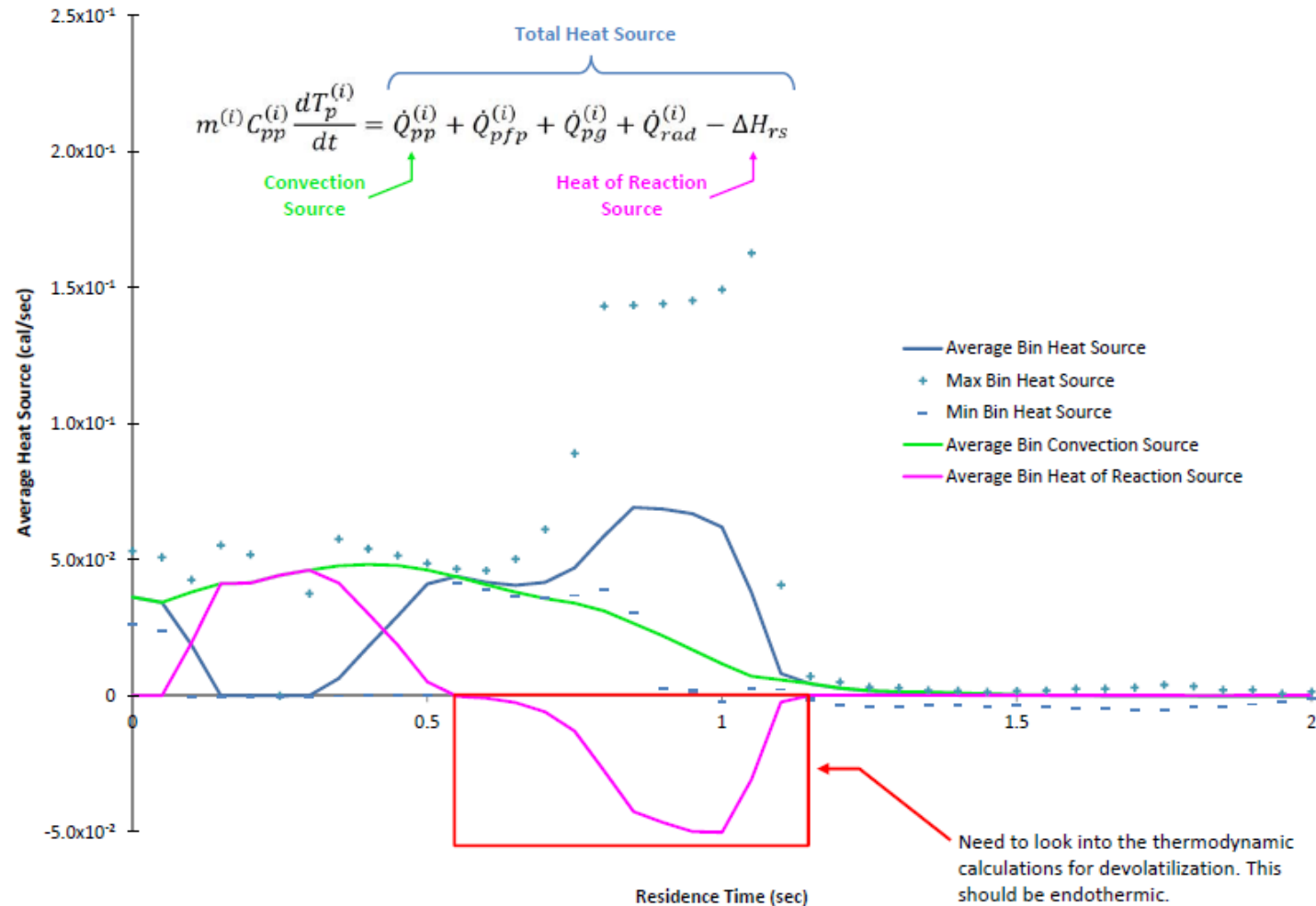
Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



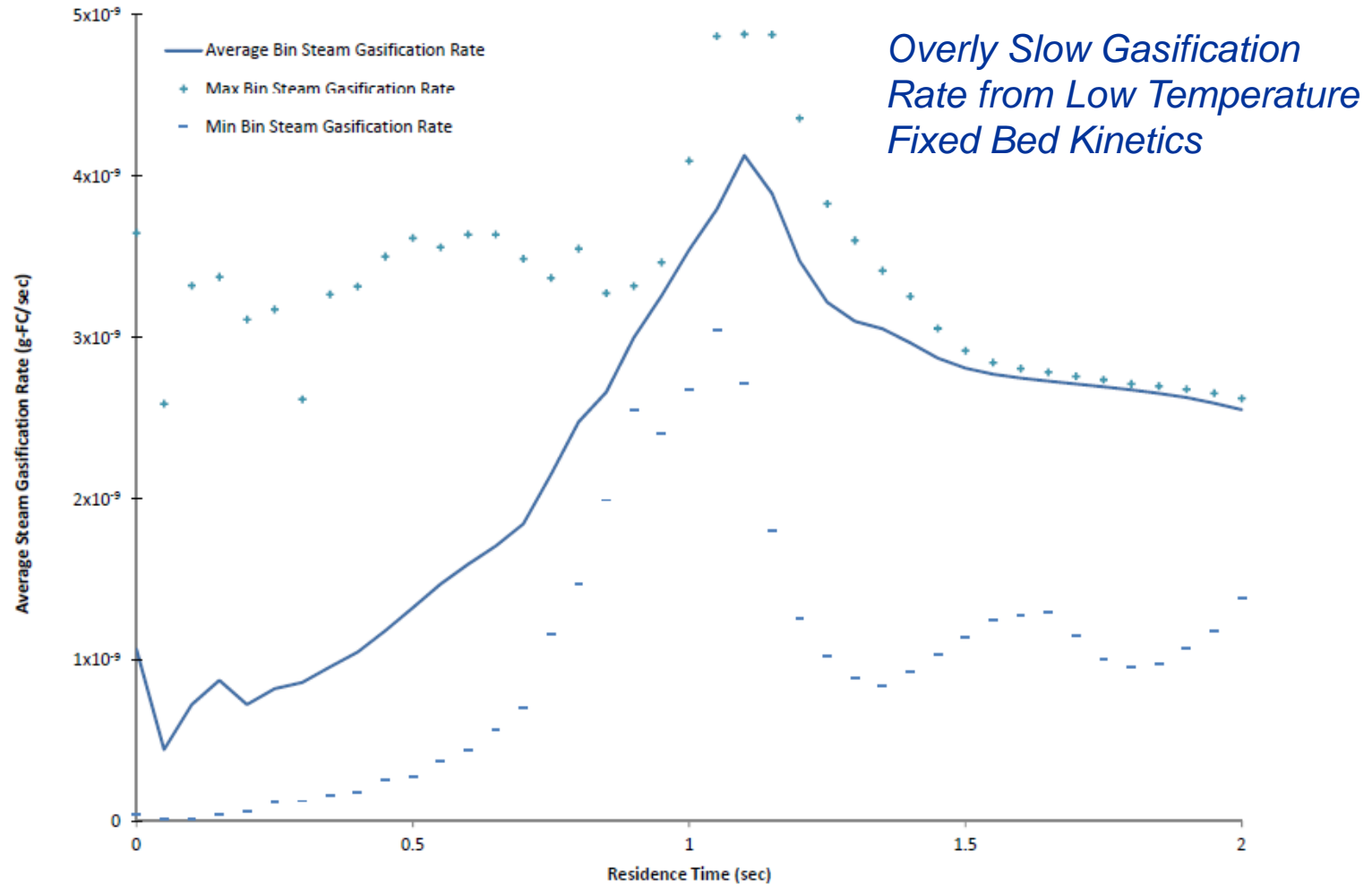
Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



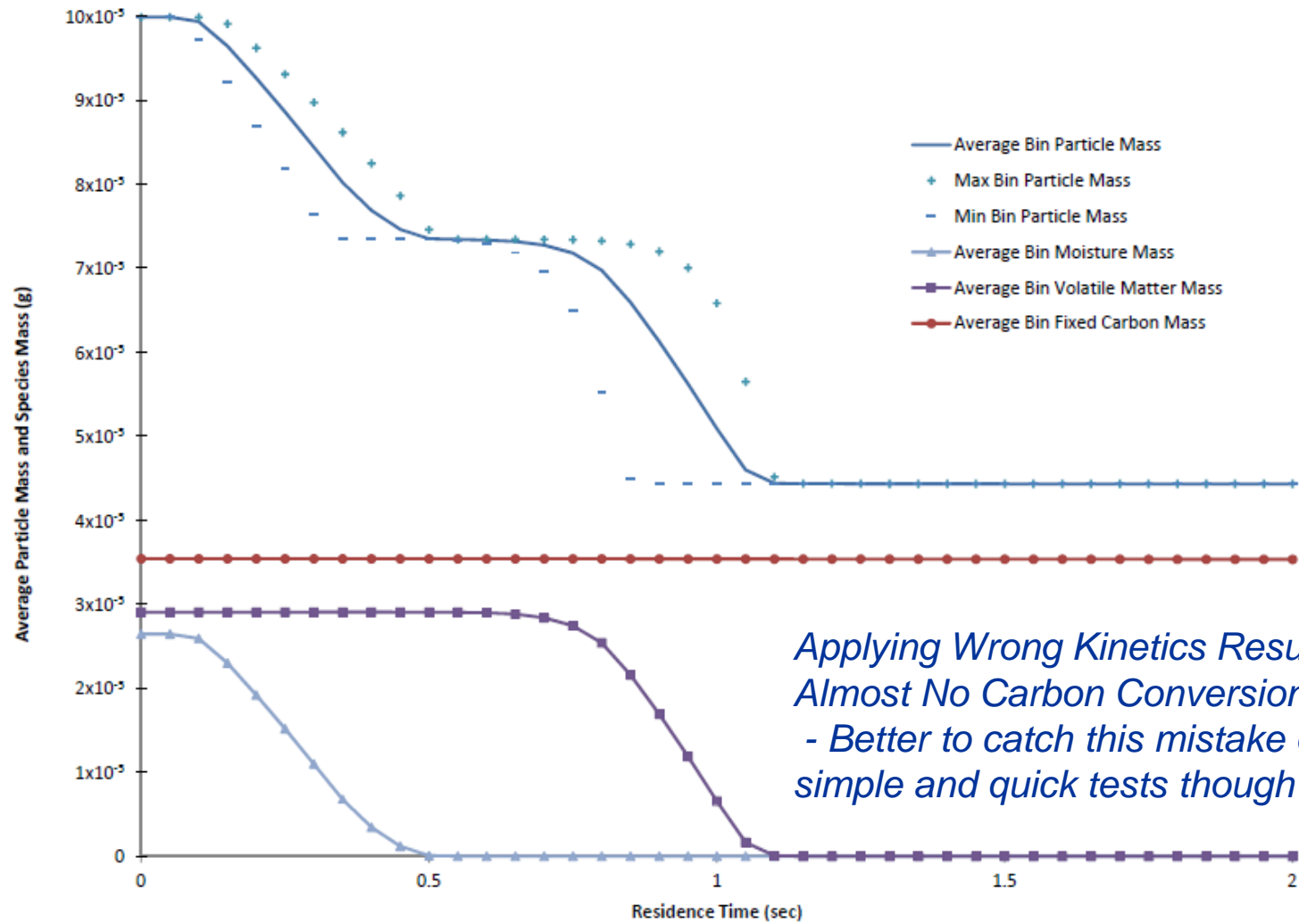
Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



Work Flow: Run CFD with C3M Chemistry

Example: Virtual Drop Tube Run in MFIX-DEM



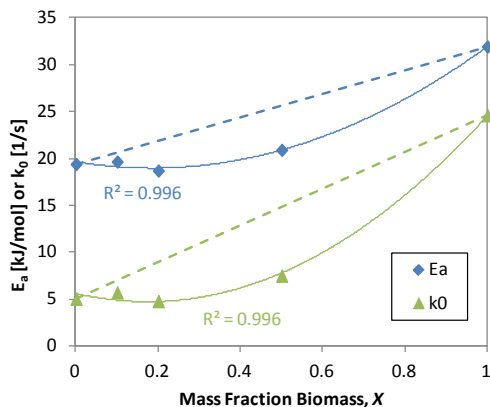
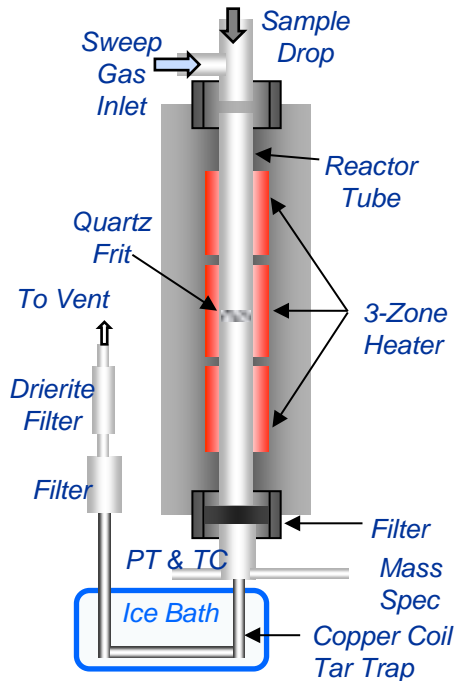
Why is C3M Needed?

- 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?

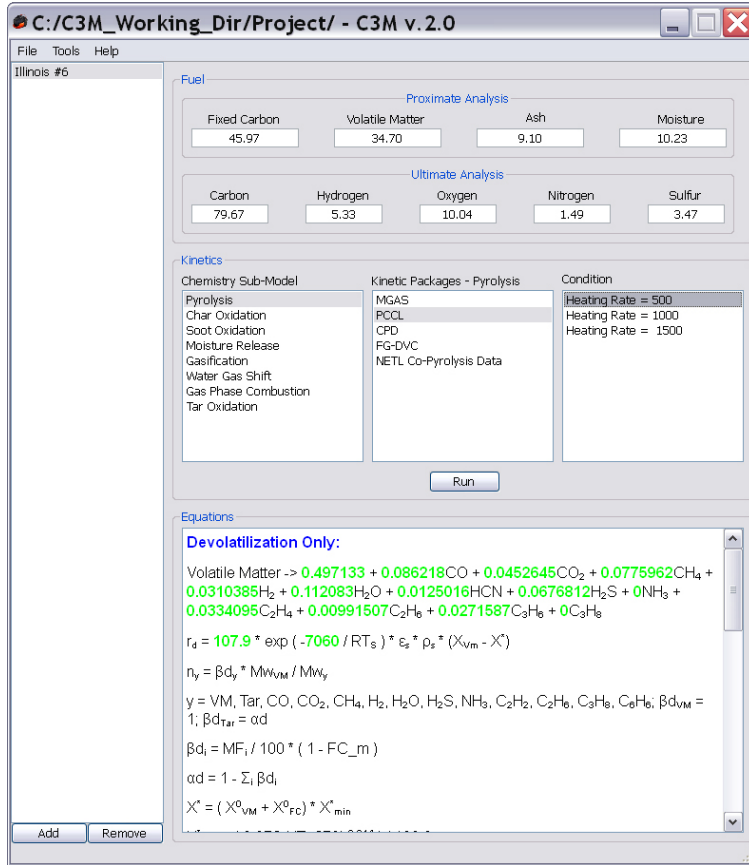
- **Direct links to kinetic data sources termed “Kinetic Packages” with appropriate licensing**
 - MGAS, PCCL, CPD, FG-DVC, and NETL HPTR Data
- **Chemical expressions and kinetic rates for gasification**
 - Moisture Release
 - Sources: MGAS and PCCL
 - Pyrolysis (Primary, Secondary, and Tar Cracking)
 - 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