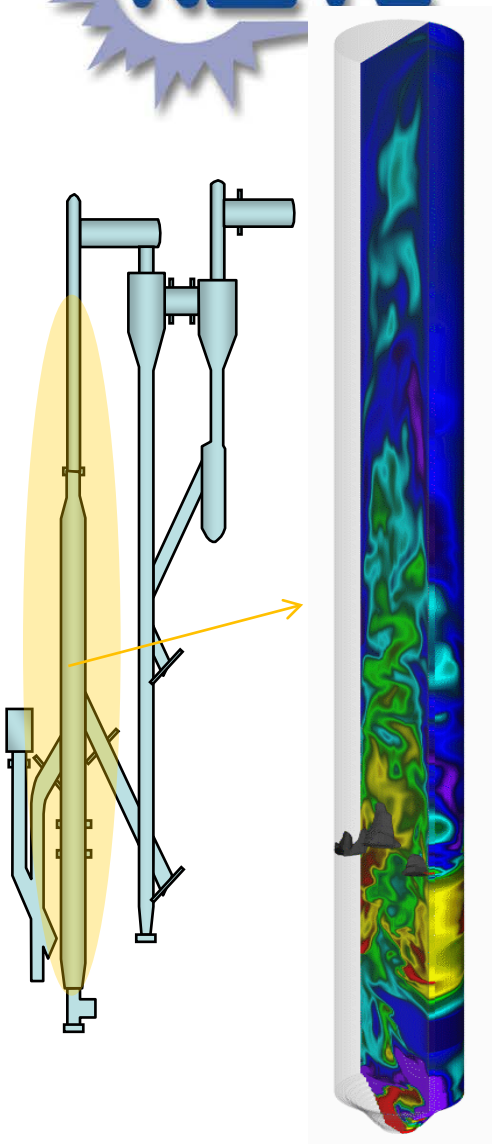
NATIONAL ENERGY TECHNOLOGY LABORATORY



Gasification Modeling Activities at the National Energy Technology Laboratory

Chris Guenther

Director Computational Sciences Division

GTC, Annual Meeting, October 28-31, 2012, Washington DC

Agenda

- **Overview of NETL's Office of Research and Development's Gasification R&D**
- **Overview of Gasification Modeling Activities Part 1**
  - Refractory Improvement
  - Conversion and Fouling
  - AVESTAR Center
- **Overview of Gasification Modeling Activities Part 2: Low Rank Coal Optimization**
  - Carbonaceous Chemistry for Computational Modeling (C3M)
  - Three Examples of Uncertainty Quantification (UQ)
    - Multiphase CFD
    - Proximate and Ultimate Analysis
    - C3M

Gasification Team R&D Structure

Gasification Team

- Refractory Improvement
- Conversion & Fouling
- Low Rank Coal Optimization
- Warm Gas Clean-up
- AVESTAR Center

Improved capacity factor for lower COE

Higher efficiency by enabling syngas heat recovery without fouling

Enable low-rank coal and mixed feed gasification performance prediction and improvements

R&D to address EPA trace metal rules

Develop IGCC training strategy and approach.

URS Carnegie Mellon PENNSTATE 1855 WestVirginiaUniversity VirginiaTech Invent the Future

Refractory Improvement: Modeling

INPUT

- Ash Data
  - chemistry
  - quantity
  - pct.
- Gasifier Conditions
  - temperature
  - gas environment

→

COMPUTER MODEL

- Thermodynamic Computations
- Computer Modeling Predictions
- Literature
- Laboratory Test Data

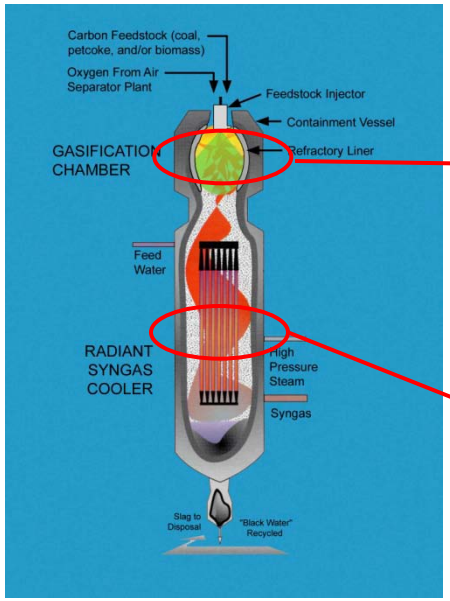
→

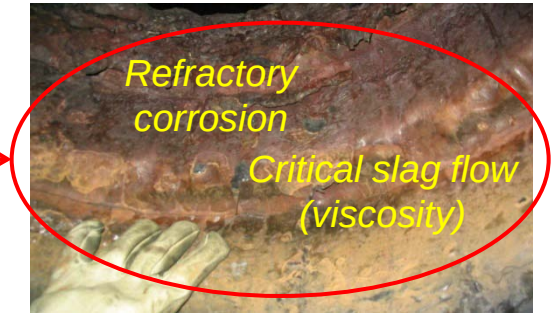
OUTPUT

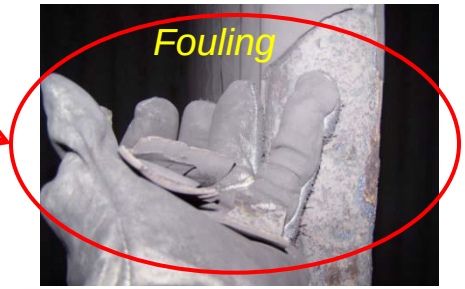
- Slag Characterization
  - melting point
  - solid/liquid/vapor phases formed
  - viscosity
- Predict and Control
  - additives to capture specific gas phases in slag
  - refractory/slag interactions
  - additives to control slag viscosity/corrosion

GOALS

- ***Primary*** *- control refractory wear and slag flow*
- ***Secondary*** - minimize syngas cooler fouling

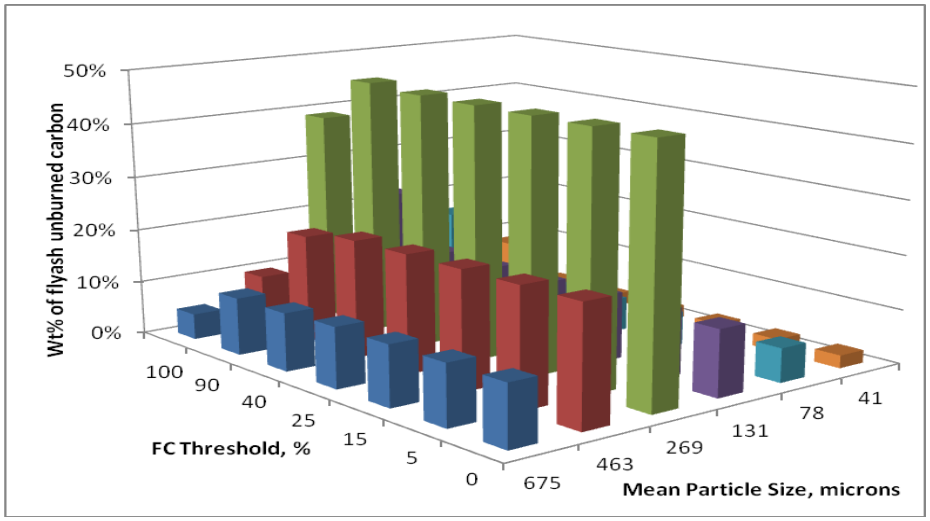






Conversion and Fouling: Modeling

Goals: Model the effects of various coal and/or petcoke fuel properties (for various density and size fractions) on unconverted carbon and syngas cooler fouling in entrained flow gasifier systems.



Objectives

- Develop heuristic spreadsheet-based reduced order model (ROM) to predict mineral matter split between slag and flyash for entrained-flow gasifiers.
- Develop sub-models for particle-slag interaction, particle fragmentation, and mineral matter chemistry (sulfur release) and implement into CFD multiphase model.

WestVirginiaUniversity

AVESTAR™ Center: Modeling

Advanced Virtual Energy Simulation Training And Research

- Mission:
  - Comprehensive *training*, *education*, and *R&D* on the efficient, safe, and reliable *operation* of *clean energy systems*
- Tools:
  - Dynamic Simulators with Operator Training Systems (OTS)
  - 3D virtual Immersive Training Systems (ITS)
- Simulators:
  - IGCC w/ CO_2 capture (OTS-3/11, ITS-2Q12)
- High-Fidelity Dynamic Model
  - Normal base-load operations
  - Mulitzonal kinetic reactor models
  - Startup, shutdown, load following
- Facilities:
  - NETL, WVU/NRCCE in Morgantown, WV
- Partners:

NETL-RUA Regional University Alliance

West Virginia University

FCS Fossil Consulting Services, Inc.

invensys

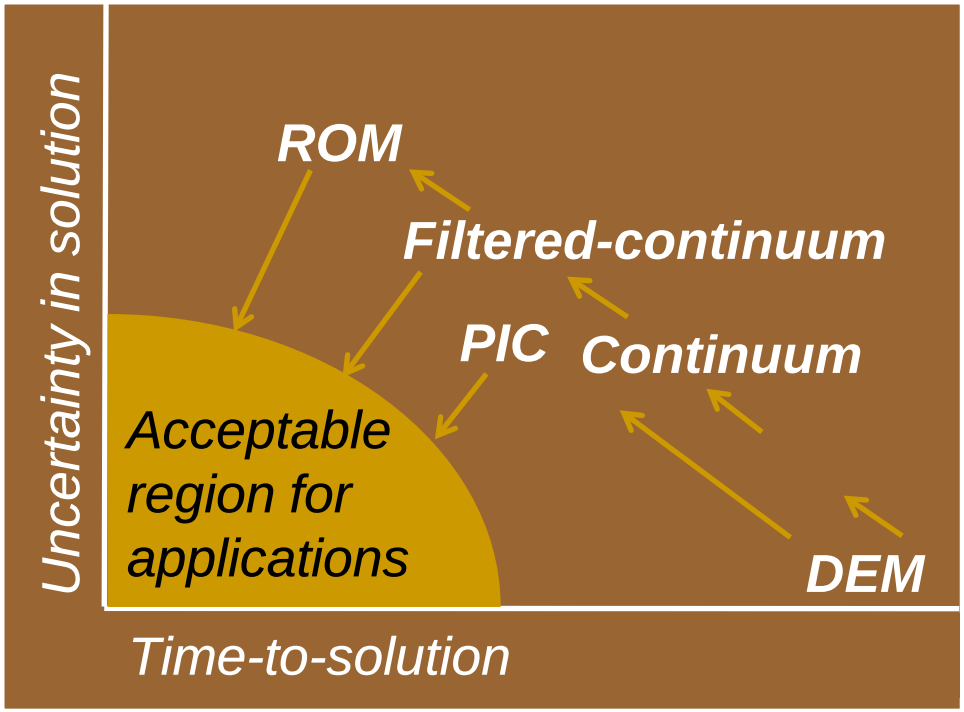
Low Rank Coal Optimization: Multiphase Models

Goal

- To develop an hierarchy of models for numerical simulations of gasifiers with a framework in place, to quantify the **uncertainty** associated with each model's predictions.

Objective

- NETL's open source suite of multiphase solvers such as MFIX-DEM, MFIX continuum, MFIX-PIC and multiphase Reduced Order Models will be used to aid in the design and optimization of operating conditions and establishing performance trends in the NCCC/TRIG.



Quantifying uncertainty, implementation of kinetic sub-models and time-to-solution are the primary needs in reacting multiphase CFD models

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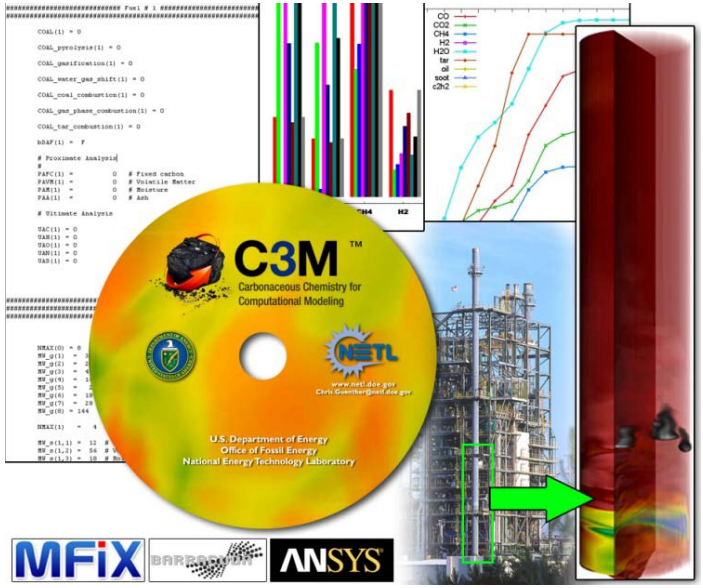
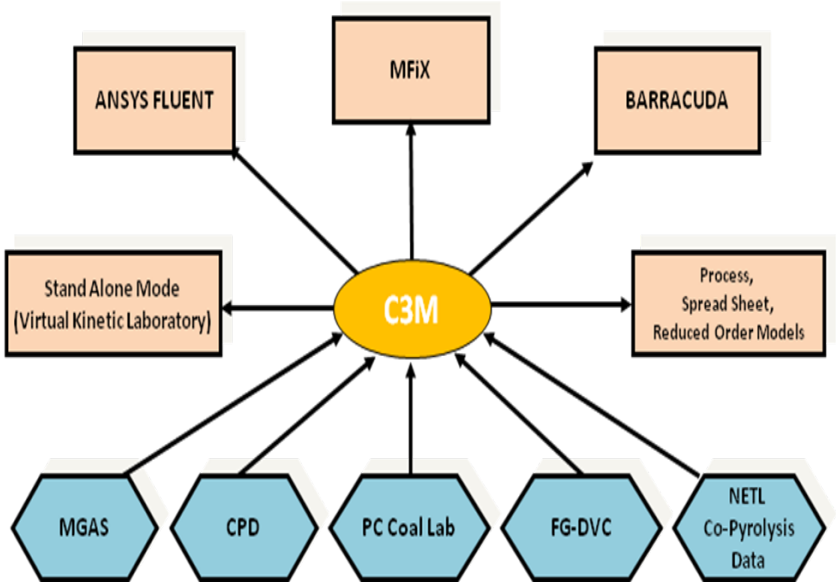
What is C3M?

- **Chemical Kinetics Management Software**
  - Provide a user friendly, comprehensive interface between reliable sources of kinetic data and reacting, multi-phase CFD models, spreadsheet or ROM's and other models
  - Provide "Virtual Kinetic Laboratory" for quickly assessing the validity of a chemical equation sets before going to full scale, expensive models





Why is C3M Needed?

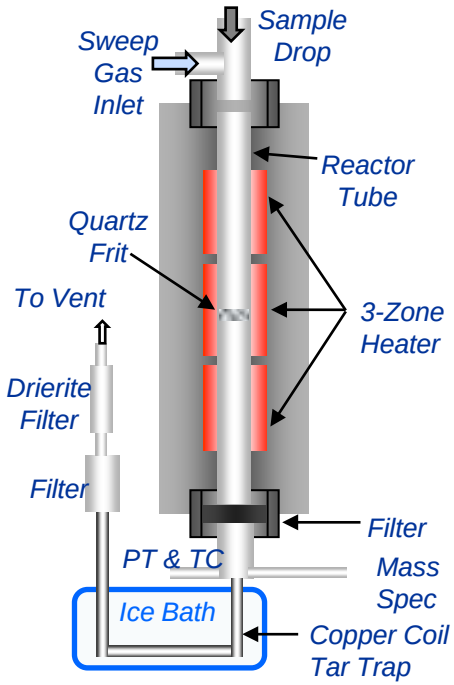
1. **Multiphase chemistry is complex (especially gasification)**
   - Real world chemistry can involve hundreds if not thousands of chemicals and reactions
   - Modelers simplify to as few as 10 or up to about 30 to capture major effects
2. **The literature availability is vast, searching for and applying 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 in a CFD or other model can cost 100's of man hours**

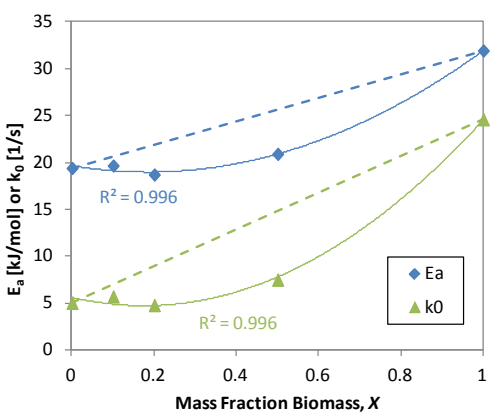
- **C3M can provide tested and validated kinetics to a modeler or researcher in minutes saving time and money in multi-phase, reacting, CFD or other model development**

What Does C3M Provide?

- **Direct links to kinetic data sources termed "Kinetic Packages" with appropriate licensing**
  - MGAS, PCCL, CPD, FG-DVC, and NETL Data
- **Chemical expressions and kinetic rates for gasification**
  - Moisture Release
  - Pyrolysis (Primary, Secondary, and Tar Cracking)
  - Char Gasification
  - Soot Gasification
  - Water-Gas-Shift
  - Gas Phase Combustion
  - Char Oxidation
  - Soot Oxidation
  - Tar Oxidation
- **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 and custom options for specific output**

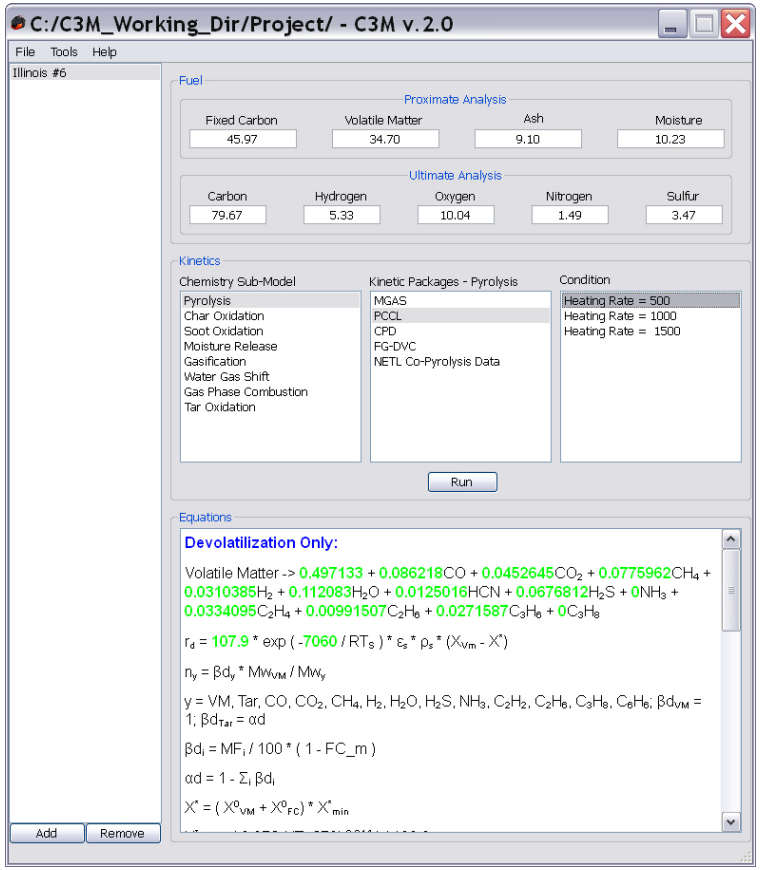
What Does C3M Provide?





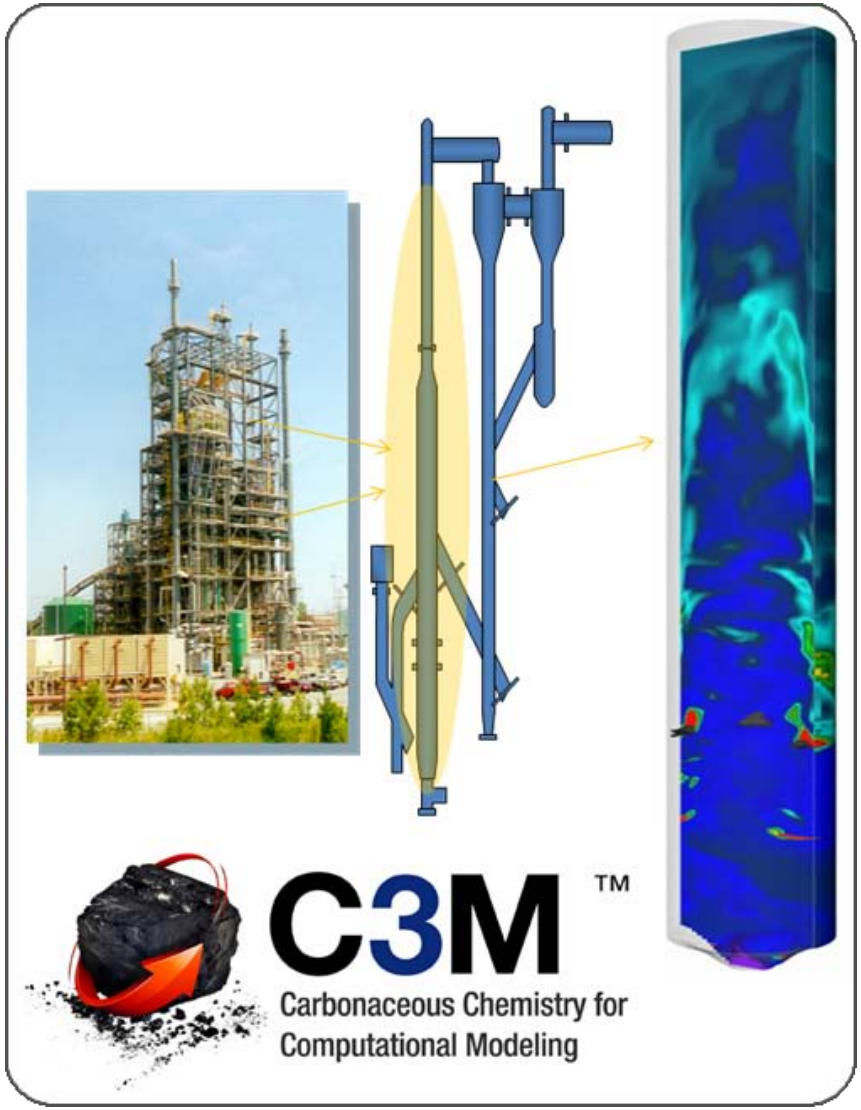
- **Kinetic Data for Fuel Flexibility**
  - Completed test campaign for southern pine and PRB for co-pyrolysis
  - Found that product gas distributions vary linearly with biomass weight fraction but kinetic rates do not
  - Data analysis is complete and reduced to a functional module within C3M
  - Testing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

What Does C3M Provide?

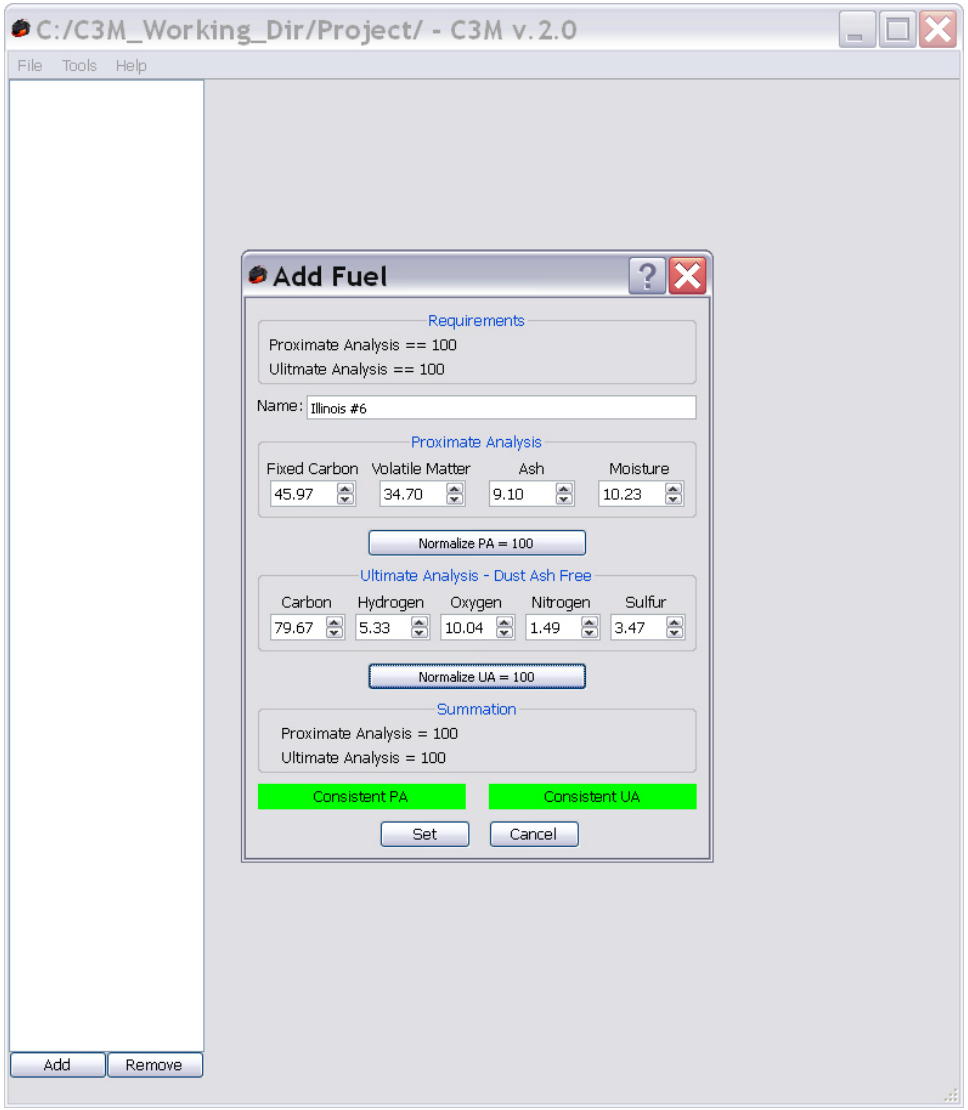


- **Easy, Intuitive, Reliable, and Graphical User Interface**
  - No cryptic text based systems
  - Intuitive work flow
  - Easy data visualization
  - Speed in building complex chemistry models
  - Reliable and tested sources of information

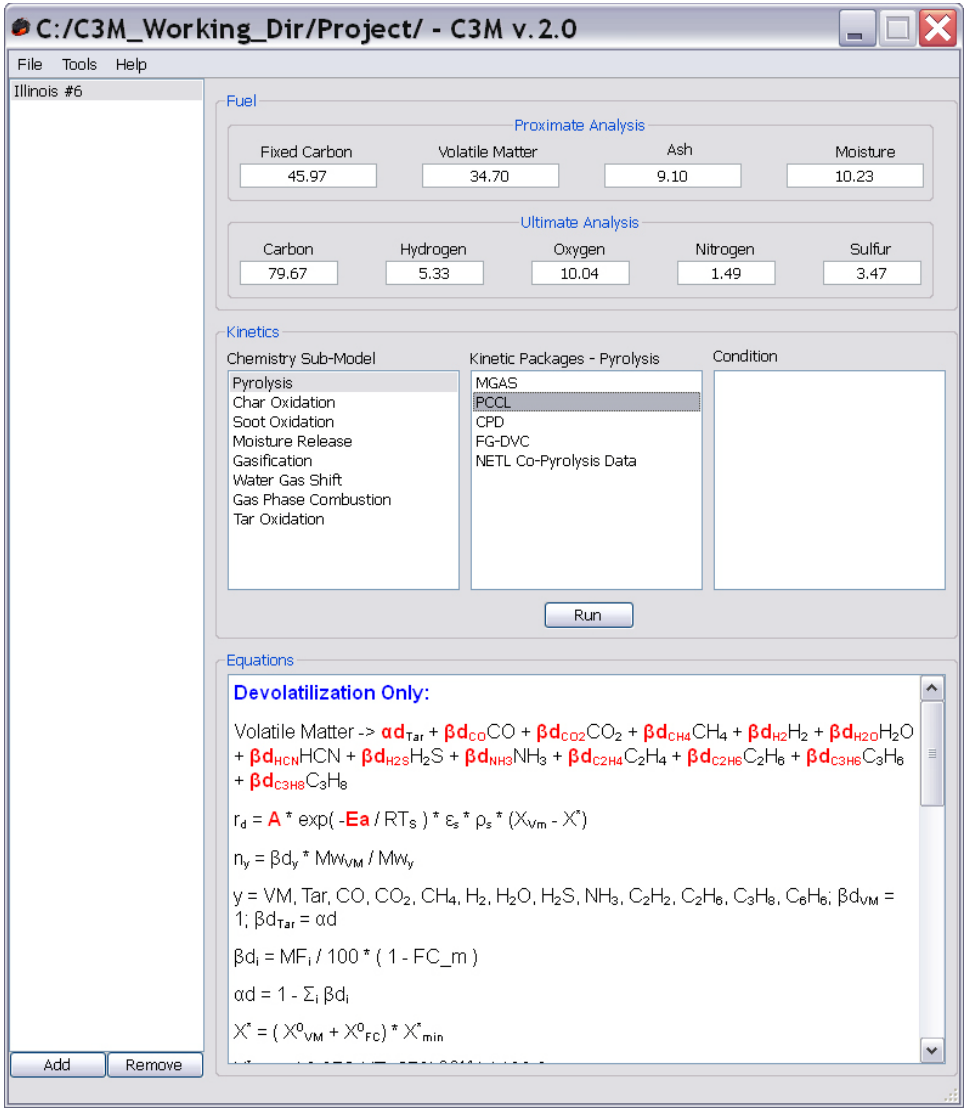
Work Flow: Open C3M



Work Flow: Input Standard Fuel Properties



Work Flow: Run All Desired Sub-Models



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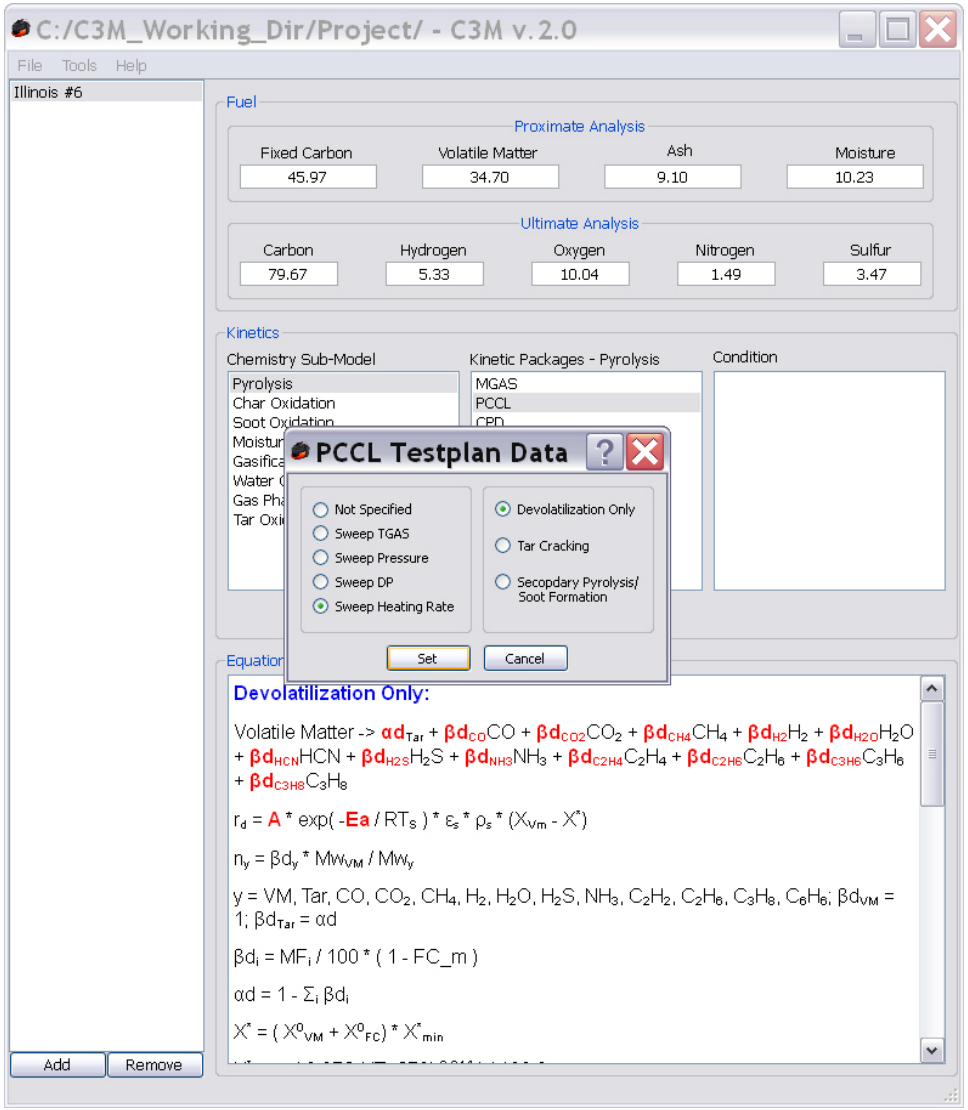
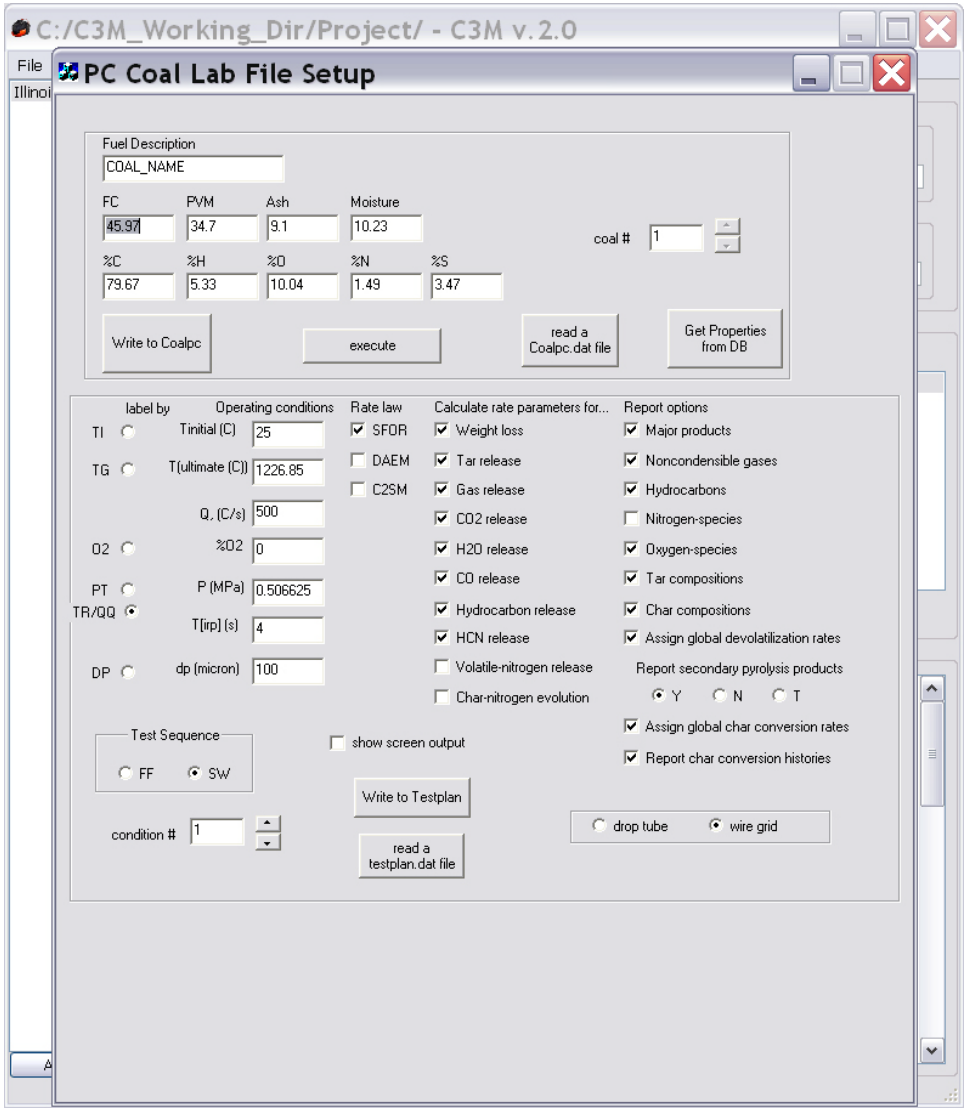
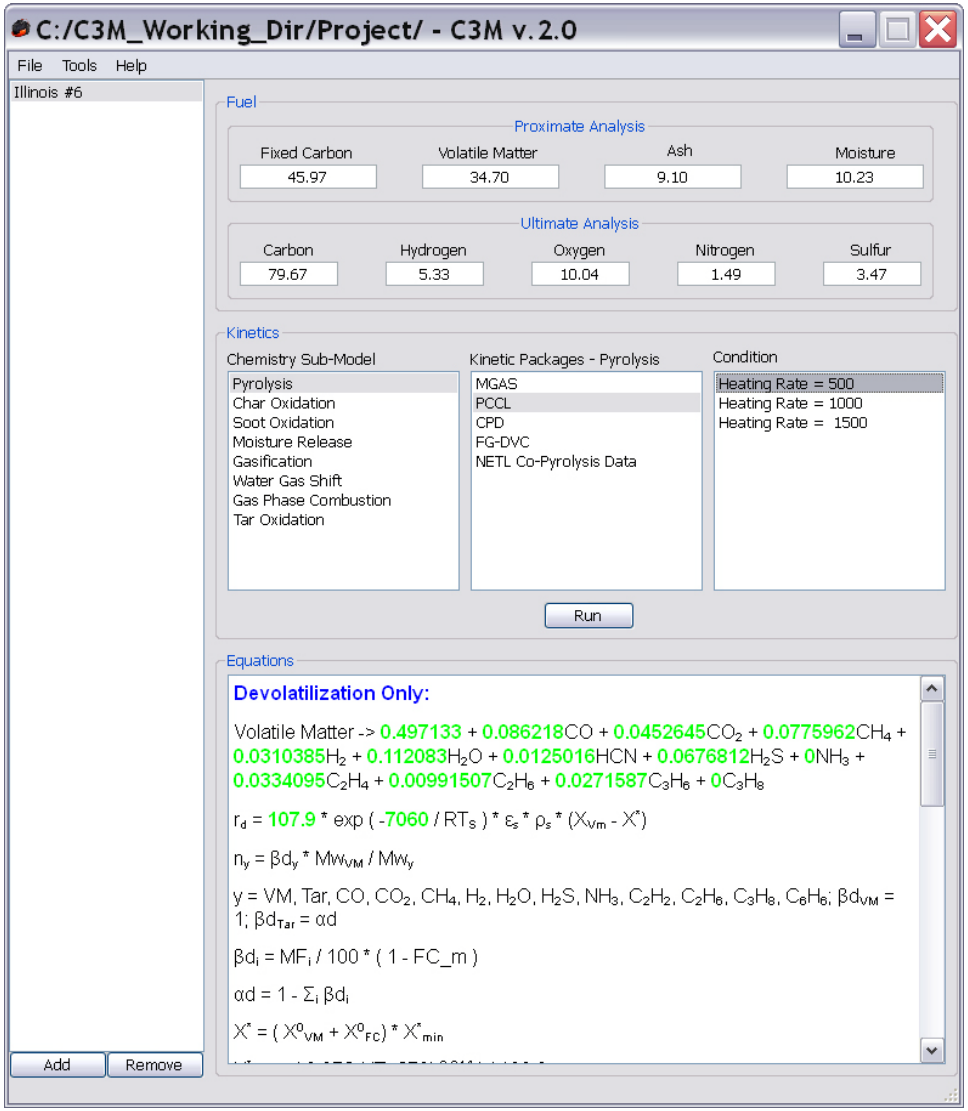


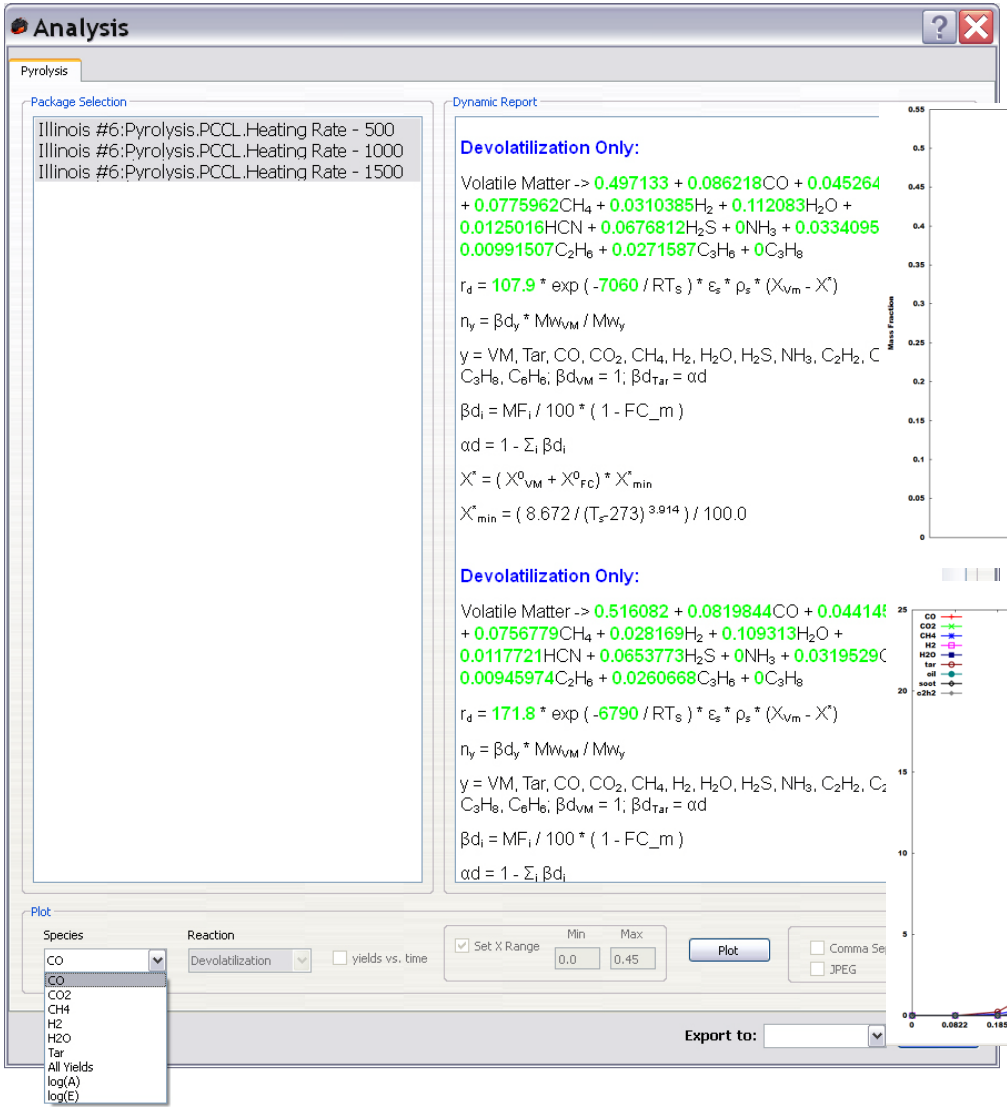
Work Flow: Run All Desired Sub-Models

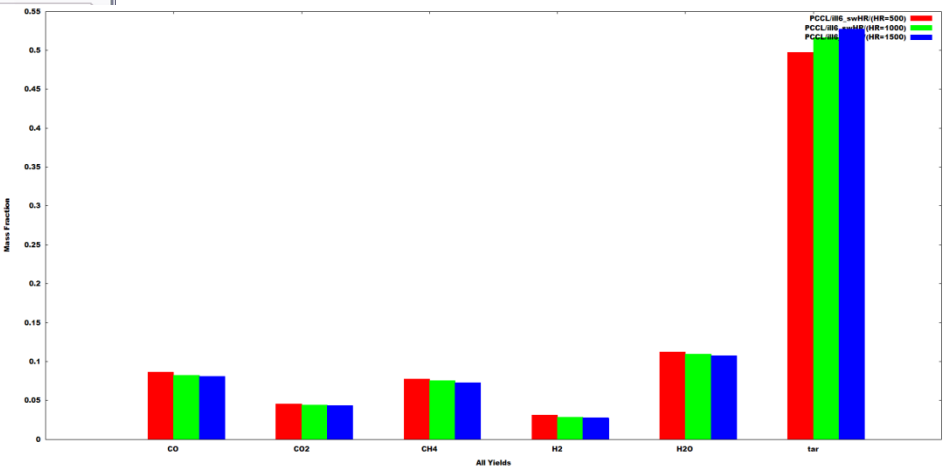


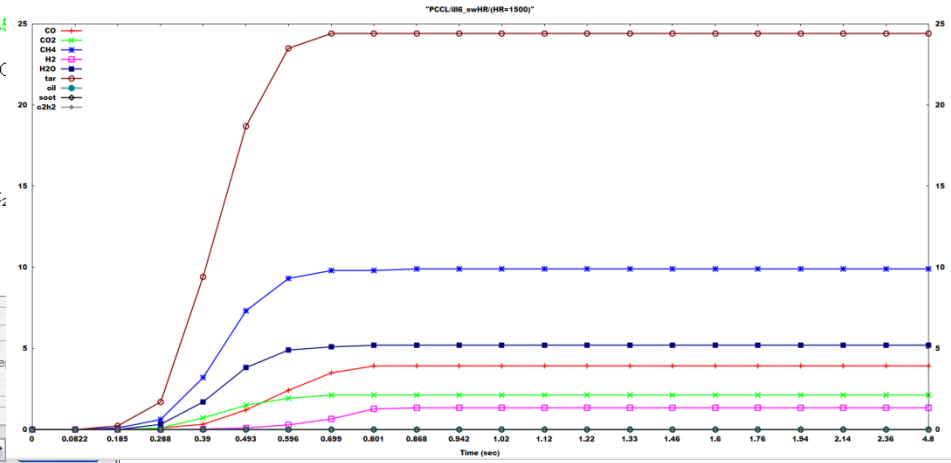
Work Flow: Run All Desired Sub-Models



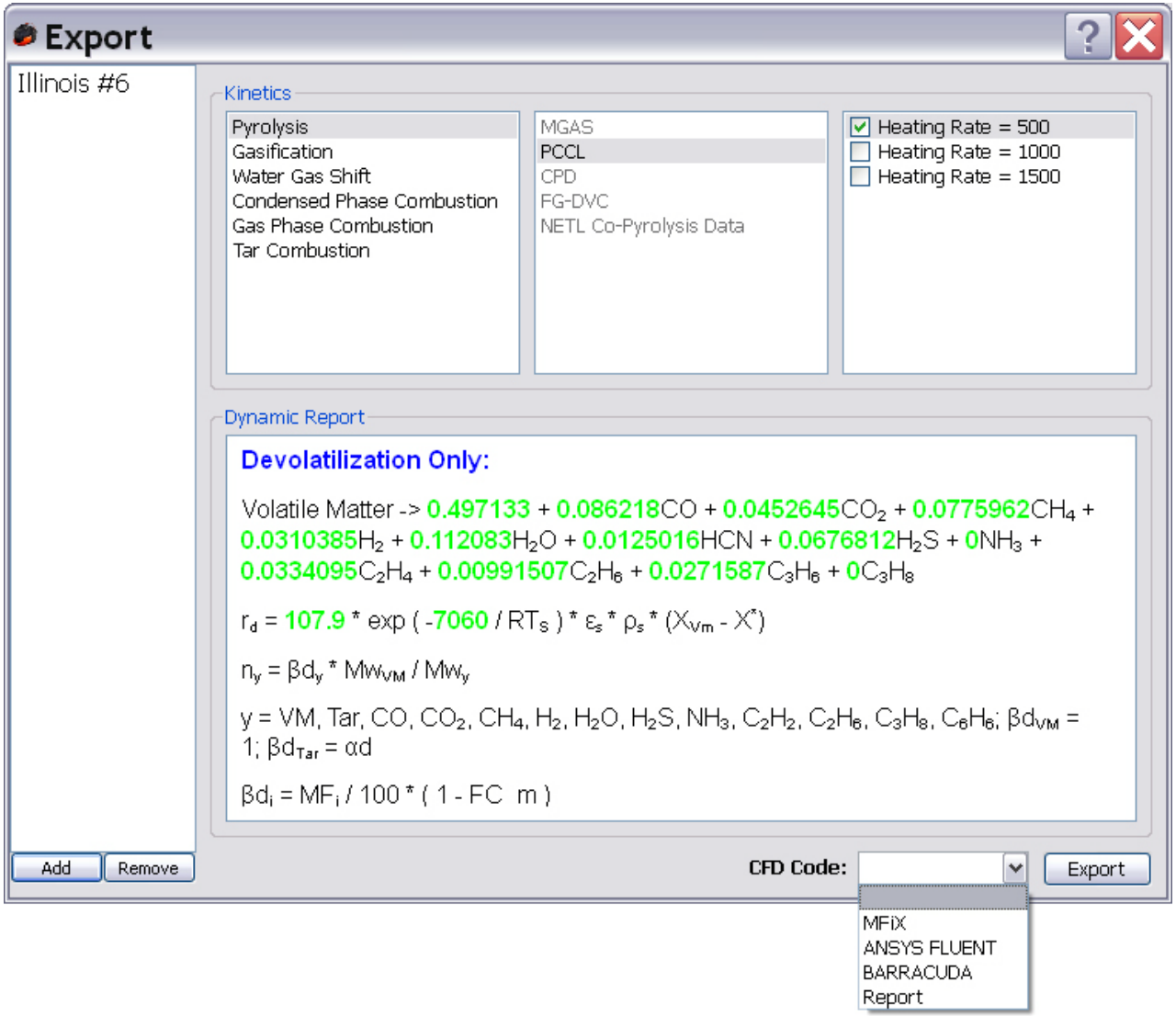
Work Flow: Compare Results



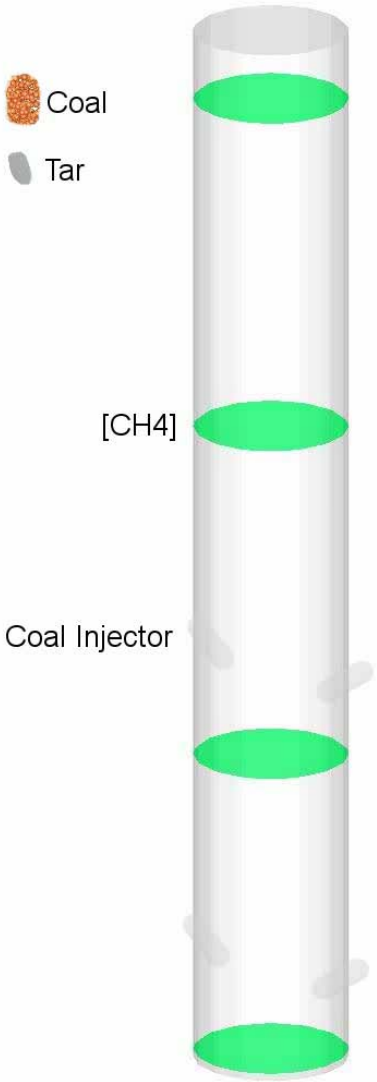


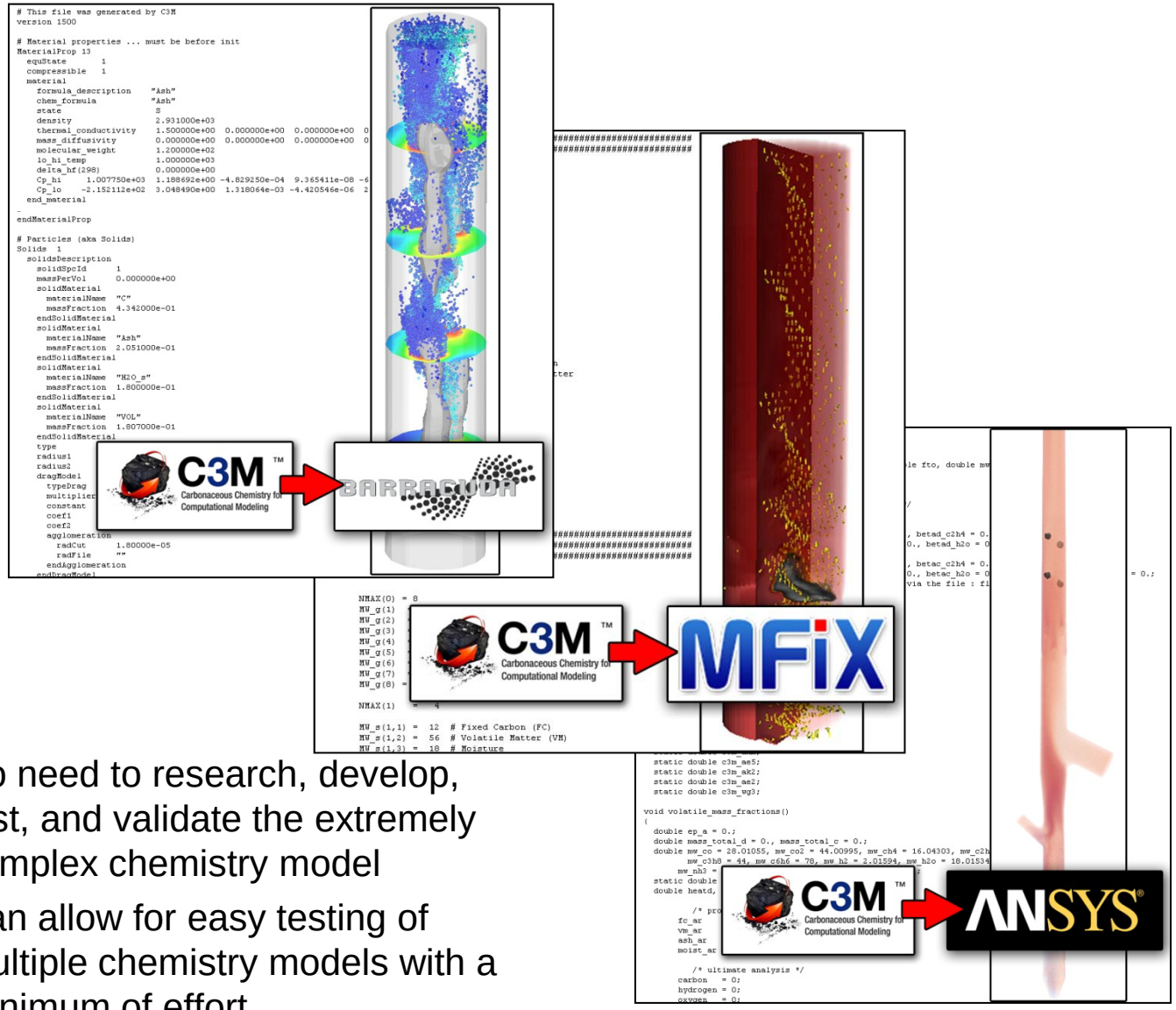


Work Flow: Select Input for Global Model



Work Flow: Generate Input Files for CFD

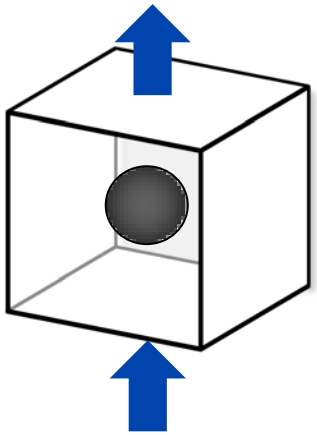


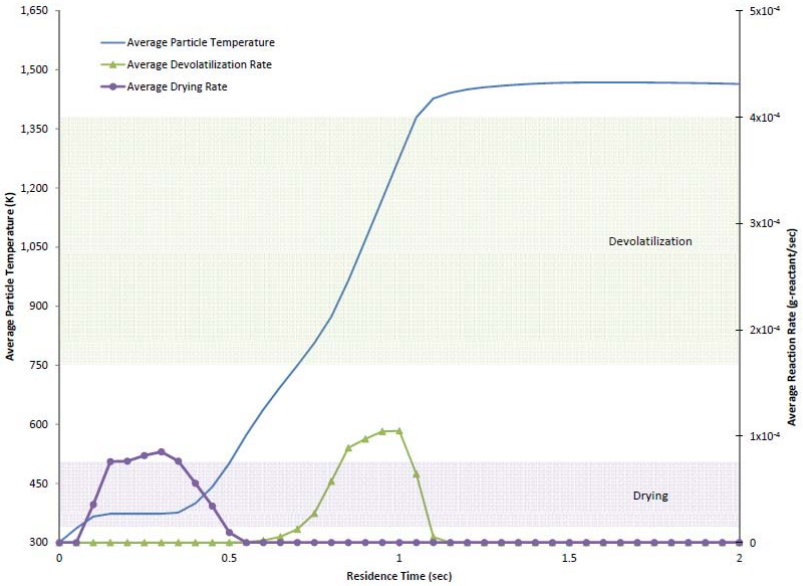


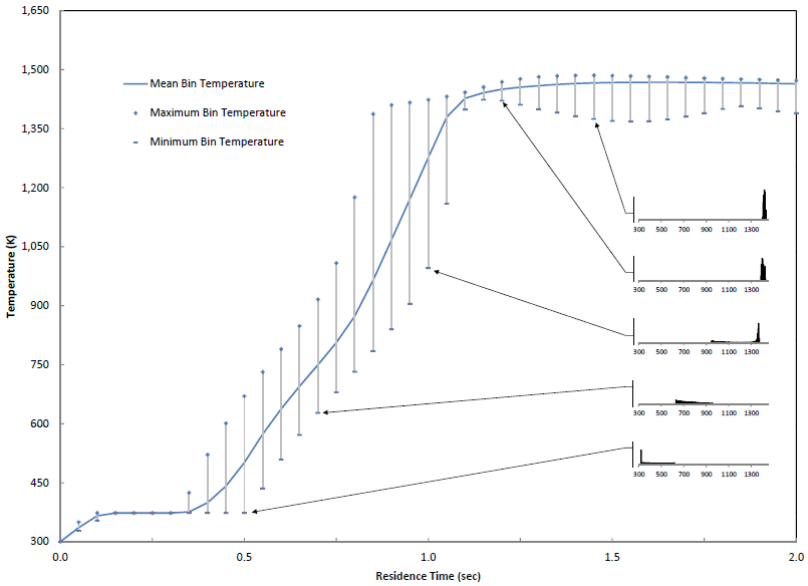
- No need to research, develop, test, and validate the extremely complex chemistry model
- Can allow for easy testing of multiple chemistry models with a minimum of effort

The Future of C3M

- **Current and Planned Activities:**
  - Release of Version 2.5 with new GUI (Fall, 2012)
  - Incorporation of a virtual drop tube and a high speed TGA through NETL's MFIX-DEM and MFIX-MPPIC models
  - Incorporating Uncertainty Quantification (UQ)

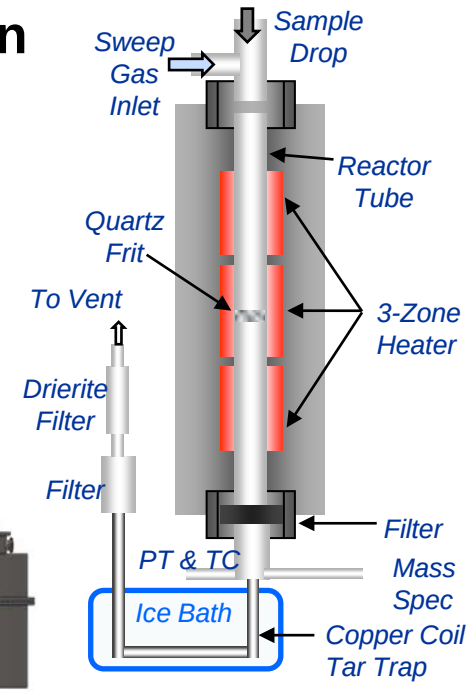


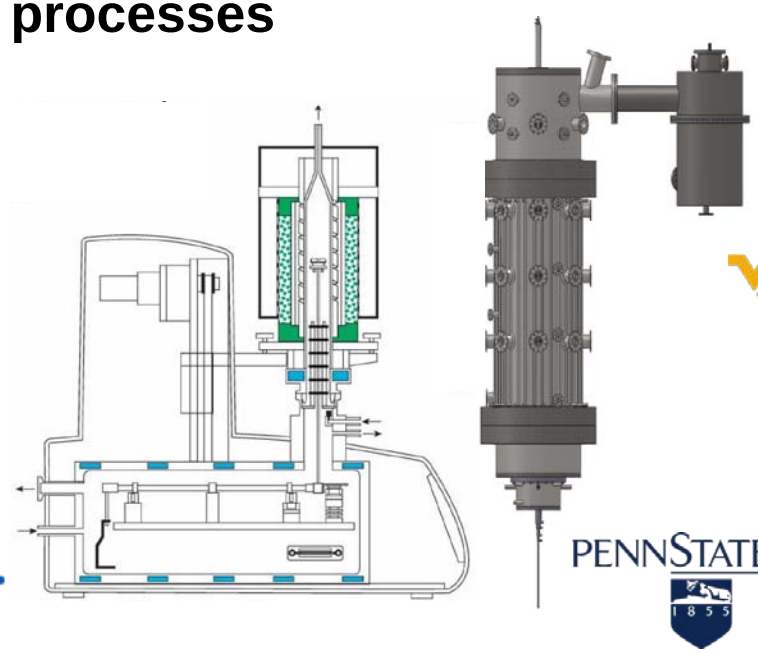




The Future of C3M

- **Increase breadth of validation test cases Gasification**
  - Include kinetics from literature
  - Expand co-gasification kinetic database
  - High pressure and temperature kinetics
  - Expand reactions for minor species (BTX, PCX)
  - Include reactions for nox/sox
- **Build modules for other processes**
  - Mercury Capture
  - CO_2 Sorbents
  - Chemical Looping
  - Oxy-combustion





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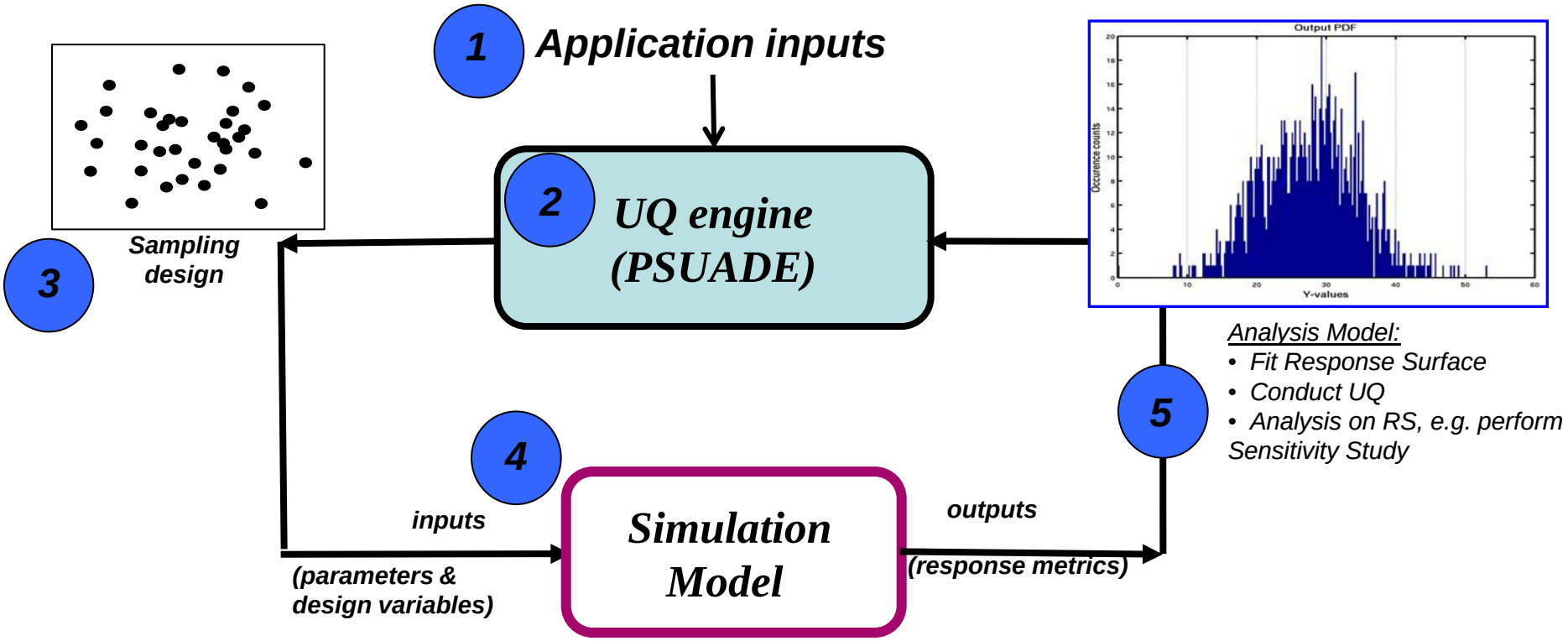
Uncertainty Quantification in Reactive Multiphase CFD Models

- **In order to accelerate gasification technology deployment from pilot scale to commercial scale, model predictions have to include the appropriate confidence interval**

- **Validation standard uncertainty from any model comes from three sources**
  - Numerical uncertainty
  - Propagation of input uncertainty through the model
  - Uncertainty in the experimental data

- **Non-intrusive techniques can be used to quantify the propagation of input uncertainty throughout the model's domain**

Input Uncertainty Propagation and Quantification – Non-intrusive method



Advantages

- *No need to modify simulation models: "black boxes"*
- *No need for analysis of the mathematical structures in the model*
- *Probe sub-model sensitivity*

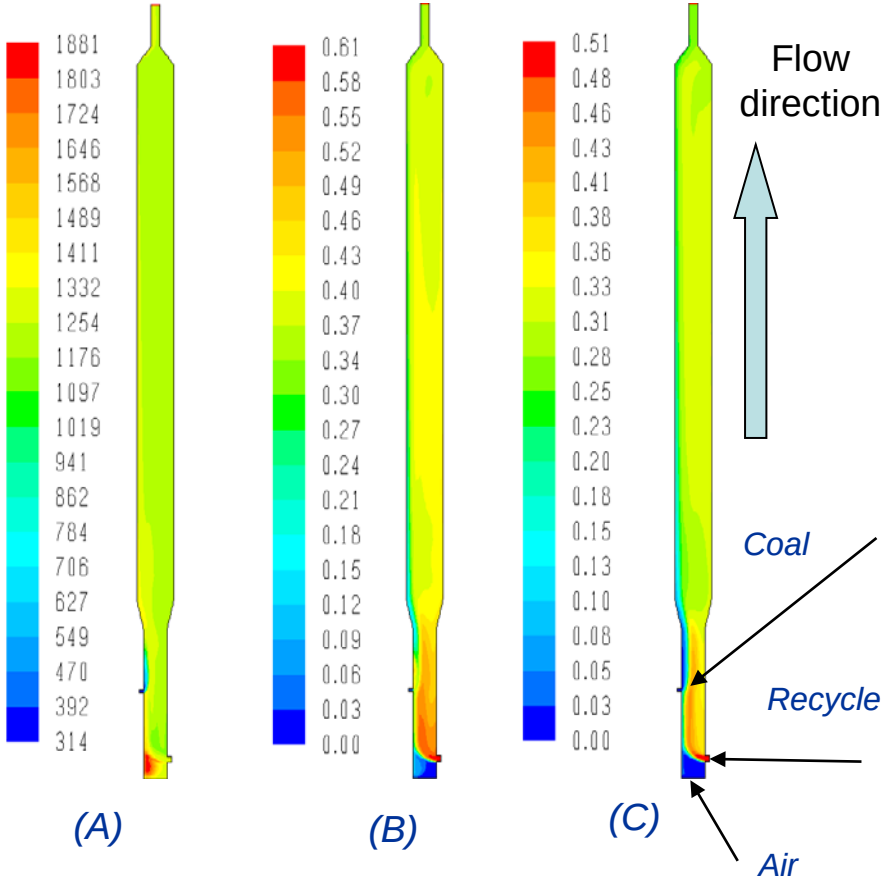
Disadvantages

- *May require large sample size for sufficient accuracy*
- *Model form uncertainty and numerical approximation uncertainty are disregarded.*
- *Assumptions on the fidelity of the surrogate model*

Example of UQ Analysis: Multiphase CFD

Goal: To characterize changes in syngas composition due to uncertainty in inflow gas temperature, in a transport gasifier simulation

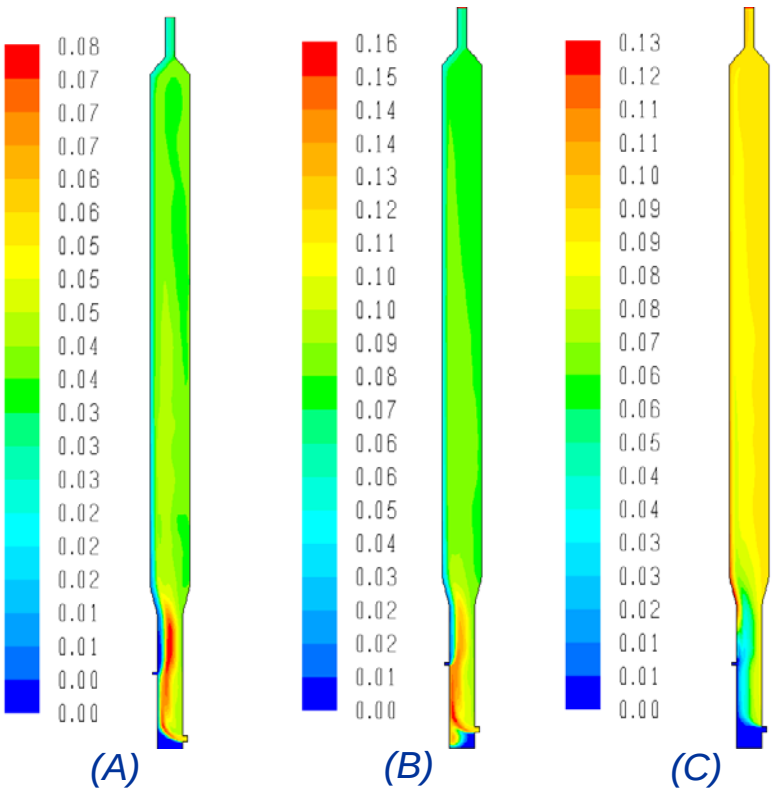
- **Kinetics generated by NETL's C3M kinetic package coupled to ANSYS/FLUENT CFD model**
- **Uncertainty in gas temperature**
  - Inflow gas temperature varying from 1100 K to 1500 K
- **Output or response variables of interest:**
  - Time averaged mole fractions (CO, H2, CH4…)
  - Reactor temperature and conversion



Time averaged temperature (A), coal volume fraction (B) and CO mass fraction (C)

Example of UQ Analysis: Multiphase CFD

1. Develop simulation design matrix by defining temperature range.
2. Conduct CFD simulation for each point in the matrix.
3. Regress response variables into a surrogate model using adjusted R^2 values.
4. Use surrogate model to perform Monte Carlo simulations on the surrogate model to explore the effect a certain temperature distribution has on response variables.
5. Sensitivity response and probability distribution functions.

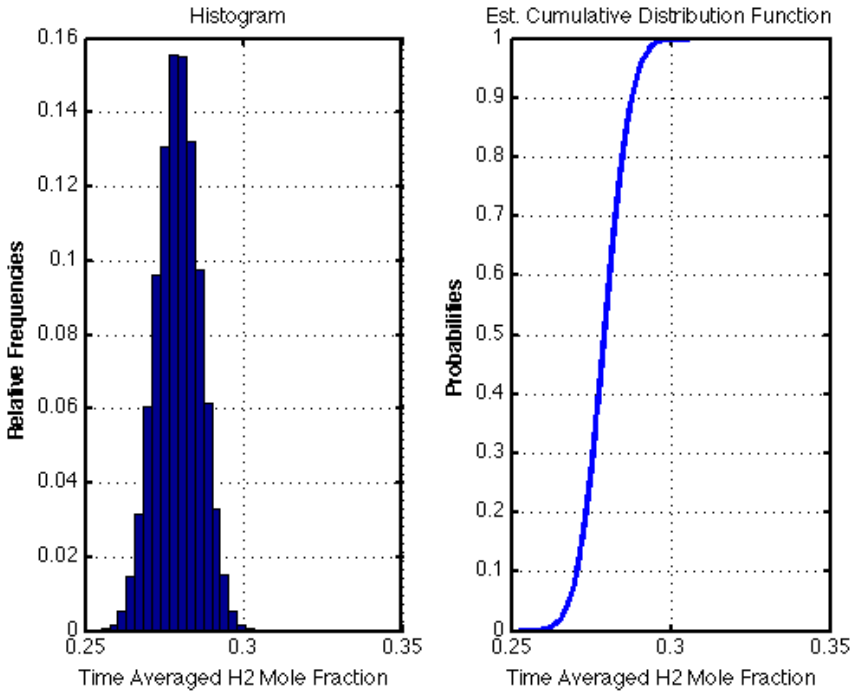


Time averaged hydrogen (A), CO_2(B) and Tar mass fraction (C)

Example of UQ Analysis: Multiphase CFD

- **The effect of uncertainty in the inlet temperature was investigated by propagating it through the surrogate model and observing the variability in the response variables.**
- **Example, the effect of inlet gas temperature on H_2 mole fraction:**

Histogram and cumulative distribution function for this test case for a normal temperature distribution using a mean of 1400K and SD of 25K



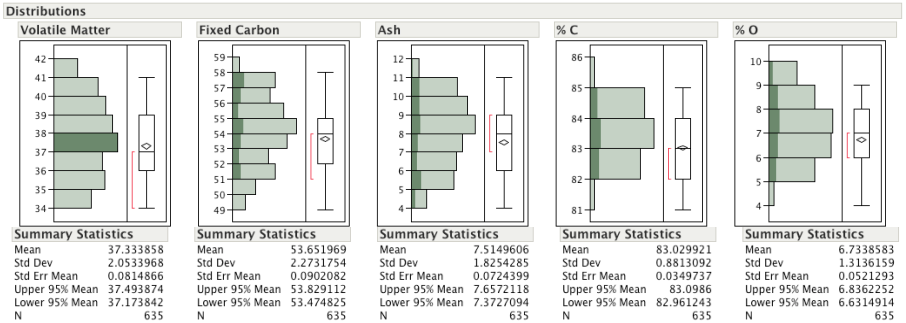
Example of UQ Analysis: Proximate and Ultimate Analysis

Coal Type: Pittsburgh 8

	Proximate Analysis:				Ultimate Analysis:				
Source:	**Volatile Matter**	**Fixed Carbon**	**Moisture**	**Ash**	**% C**	**% H**	**% O**	**% N**	**% S**
Ref #1	33.50	57.70	1.00	7.80	84.20	6.10	6.60	1.50	1.60
Ref #2	37.81	52.07	1.08	8.90	84.21	5.58	4.96	1.53	3.86
Ref #3	35.40	56.30	1.40	6.90	82.90	5.60	7.70	1.60	2.20
Ref #4	35.26	55.63	1.55	7.56	82.19	5.52	8.61	1.65	2.03
Ref #5	41.10	50.02	2.02	6.86	82.47	5.47	7.76	1.70	2.60
Ref #6	40.89	49.76	1.94	7.41	82.30	5.56	7.92	1.71	2.51
Ref #7	39.30	49.00	1.00	10.70	81.43	5.21	9.51	1.59	2.27
Ref #8	35.66	55.44	1.66	7.24	83.18	5.69	5.84	1.55	3.73
Ref #9	33.52	57.69	1.00	7.79	83.70	5.98	4.26	1.53	4.53
Ref #10	36.41	57.69	1.87	4.03	84.70	5.40	7.26	1.71	0.93
Mean	36.89	54.13	1.45	7.52	83.13	5.61	7.04	1.61	2.63
Std Dev	2.79	3.55	0.41	1.67	1.06	0.26	1.63	0.08	1.11
Max	41.10	57.70	2.02	10.70	84.70	6.10	9.51	1.71	4.53
Min	33.50	49.00	1.00	4.03	81.43	5.21	4.26	1.50	0.93

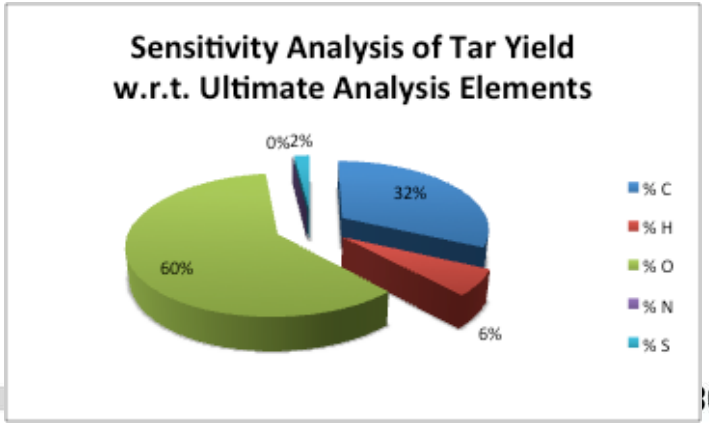
(1) Literature survey for available proximate analysis (PA) and ultimate analysis (UA) data for Pitt #8

(2) Samples generated to reflect the uncertainty in PA and UA.



(3) The samples generated are then simulated in C3M to observe the effect of input variability on the quantities of interest such as CO yield, tar yield or reaction rates.

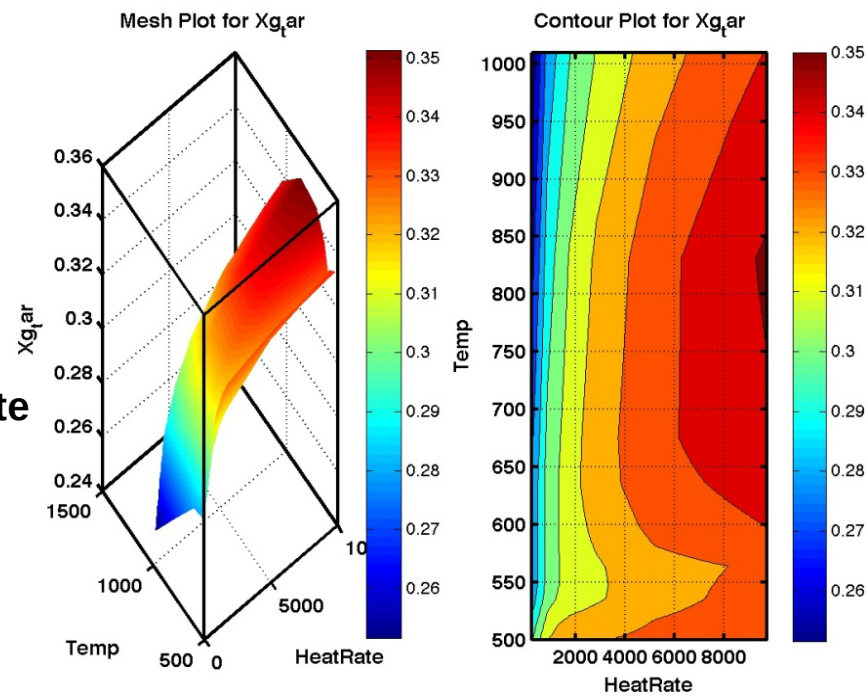
(4) Sensitivity analysis performed using the results to understand the effect of uncertainty in ultimate analysis elements on yield or reaction rates



Example of UQ Analysis: C3M

Pyrolysis gas yield response to Heating Rate, Temperature, and Pressure within C3M

- **Uncertain input parameters**
  - Heating rate (C/s) [200 – 9727]
  - Temperature (C) [500 – 1010]
  - Pressure (kPa) [861 – 3447]
- **Response surfaces for volatile gases are generated**
- **Conduct Monte Carlo simulations to generate PDFs for input parameters:**
  - 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 Direct Monte Carlo simulations on C3M and Monte Carlo simulations via surrogate model**



Response surface for propagating input uncertainty in tar pyrolysis process

Example of UQ Analysis: C3M

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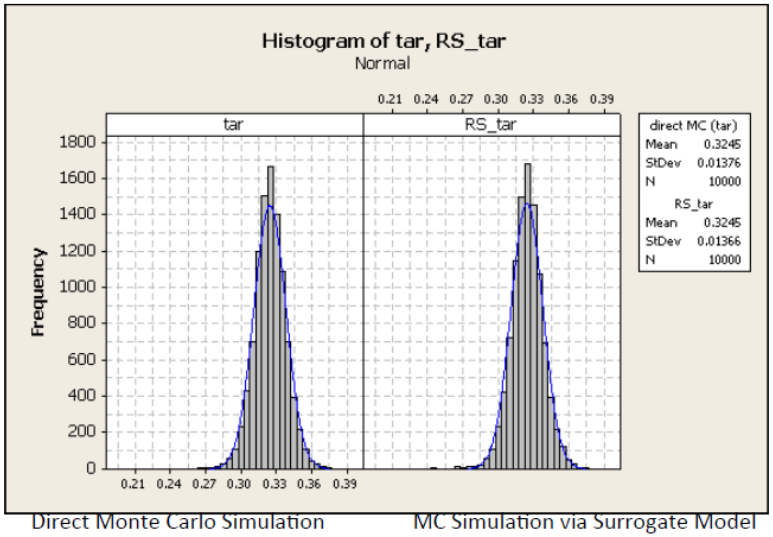
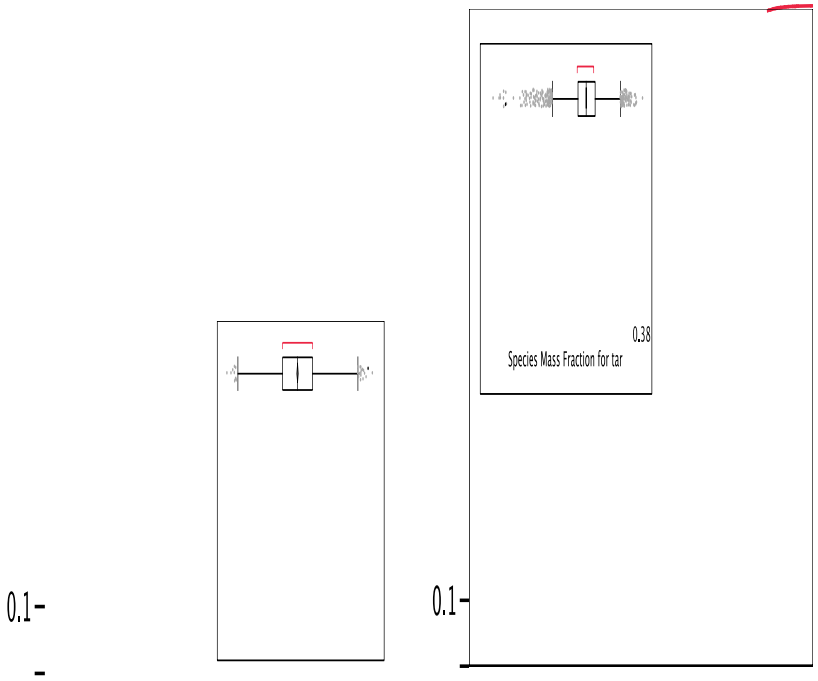


No major differences in the output parameters between direct MC simulation and MC simulation via surrogate model



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

Example of UQ Analysis: C3M

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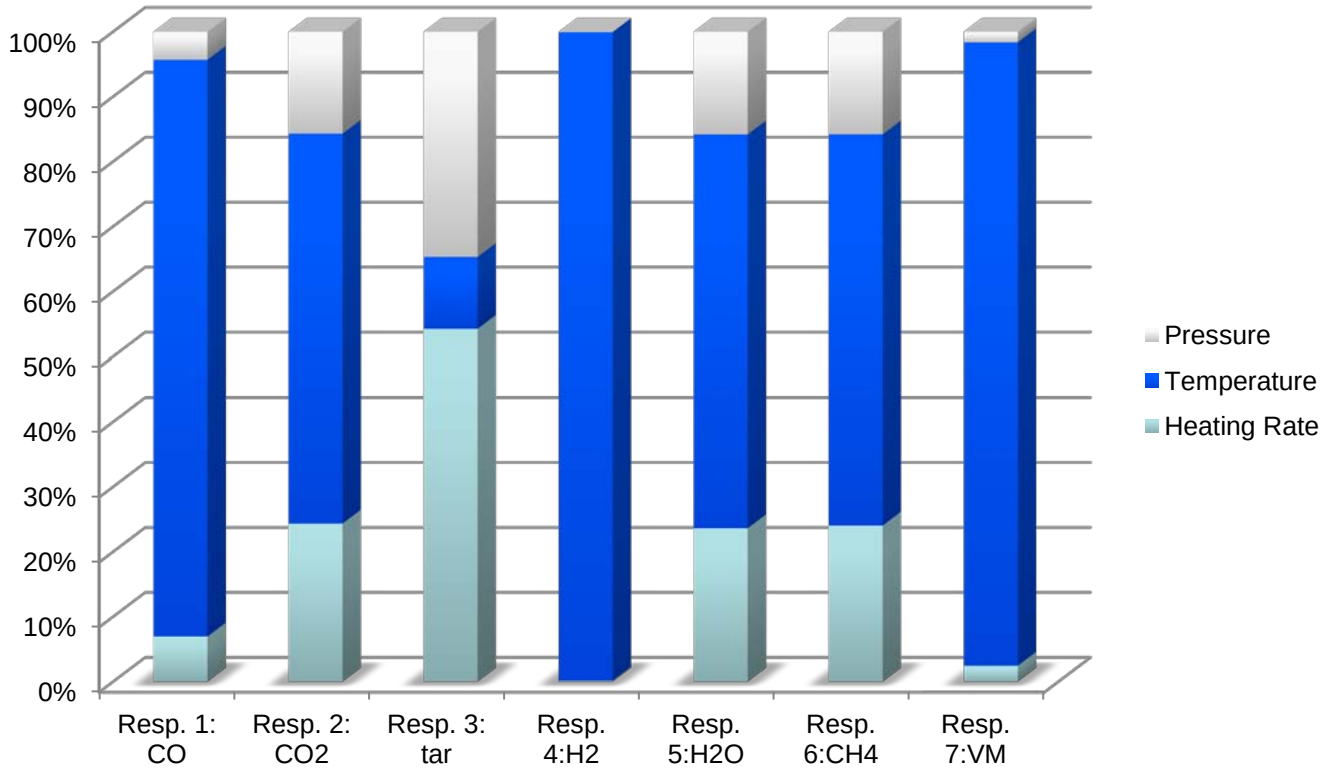
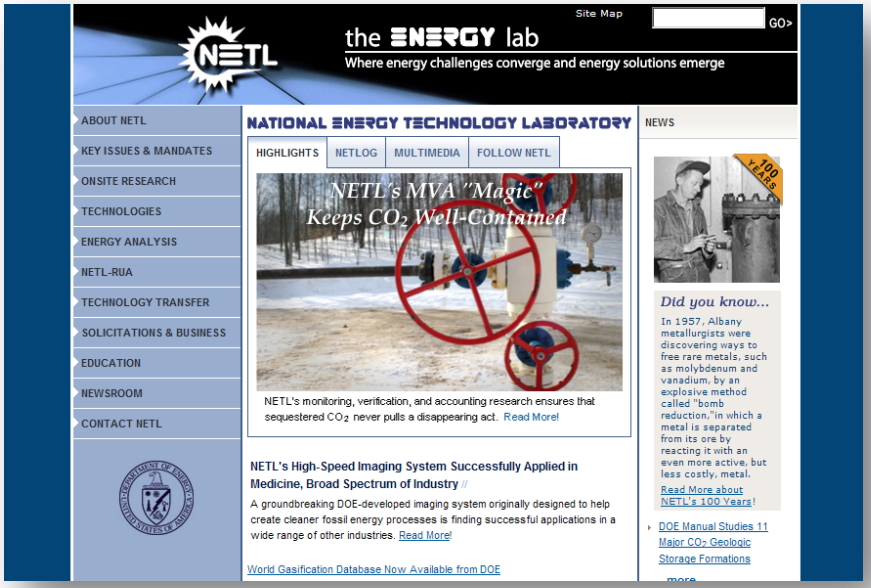
Sensitivity of Gas Products to Input Variables



Summary

- **Carbonaceous Chemistry for Computational Modeling (C3M)**
  - Gasification kinetics are fully integrated with leading multiphase CFD models
  - Provides a virtual kinetic laboratory
- **UQ can help answer questions about the uncertainty in**
  - CFD and kinetic model predictions
  - Parameters in sub-models
  - Reactor operating conditions
  - Changes in fuel properties
- **Computational models being developed cover a broad range of application for the gasification industry (refractory, slag, fouling, CFD, kinetics, IGCC training, etc..)**

Thank You!



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