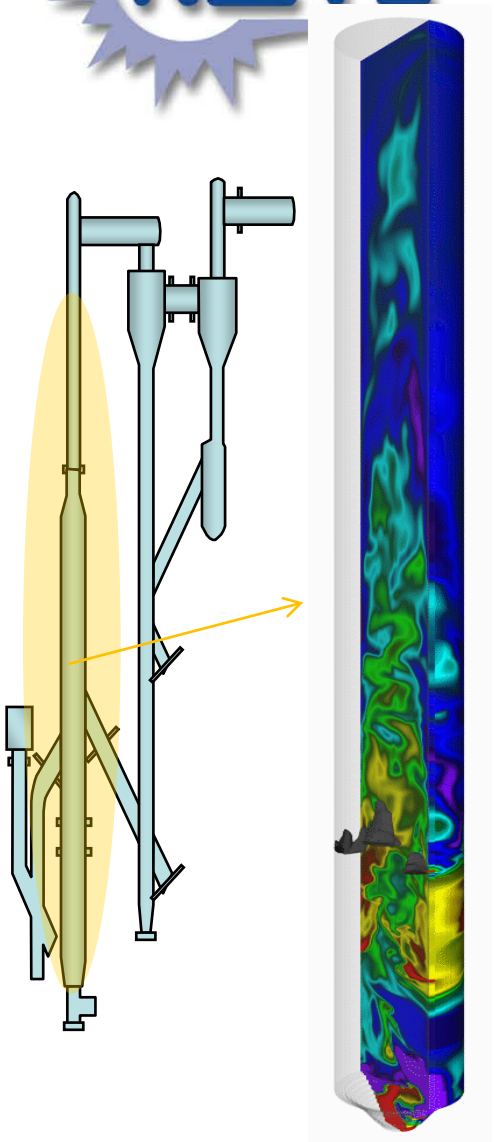
NATIONAL ENERGY TECHNOLOGY LABORATORY



Multiphase Flow Science

Chris Guenther, Director Computational Science Division

RUA Spring Meeting, Morgantown, WV March 2013

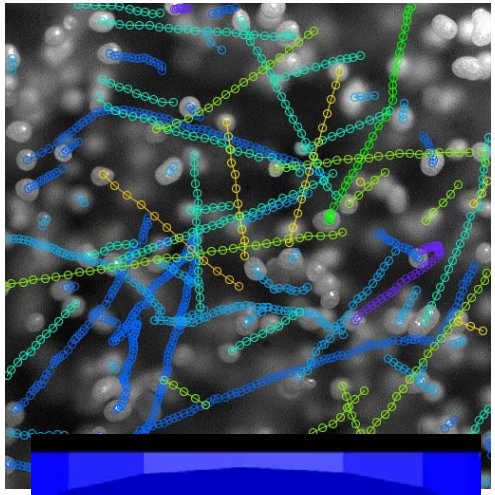
NETL's Multiphase Flow Science Team

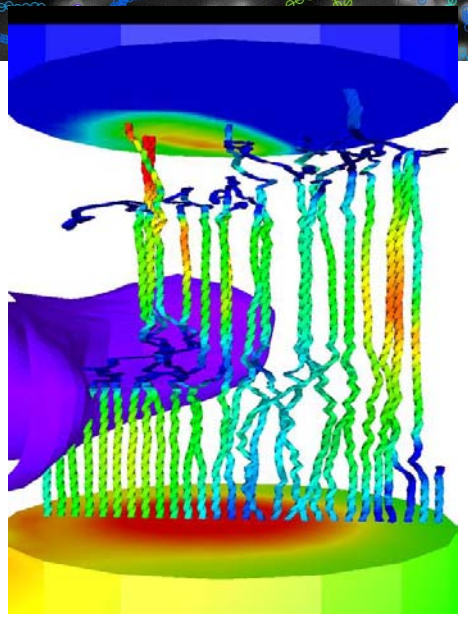
- **The Multiphase Flow Science Team develops physics-based simulation models to conduct applied scientific research.**
  - Development of new theory
  - Extensive on-site and collaborative V&V efforts and testing
  - Engages in technology transfer
  - Applies the models to industrial scale problems.

Why is Multiphase Flow Science Needed?

- Industry is increasingly relying on multiphase technologies to produce clean and affordable energy with carbon capture.

- Unfortunately, the presence of a solid phase reduces the operating capacity of a typical energy device from its original design on average by 40% [1]. This is in stark contrast to the chemical industry where devices are typically single phase and operate at 90% or higher of design capacity.



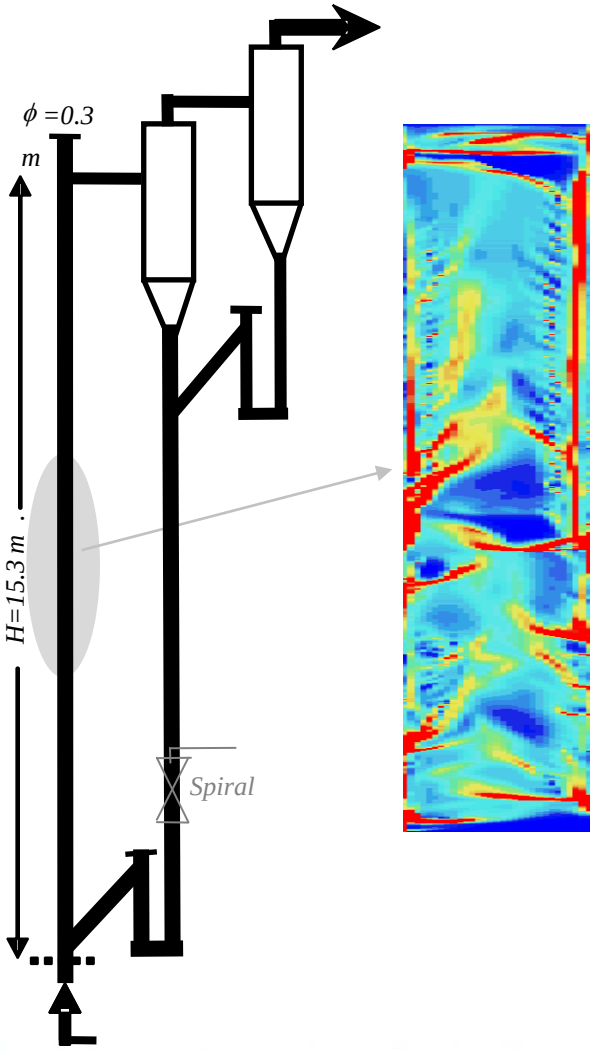


[1] Merrow E., “Linking R&D to problems experienced in solids processing“, Rand Report pp.14-22, 1985.

NETL Advancing the State of the Art in Multiphase Flow Science

- Through establishing an in-house core competency and collaboration with internationally-recognized experts and disseminating the knowledge by providing an open-source research platform MFiX www.mfix.netl.doe.gov

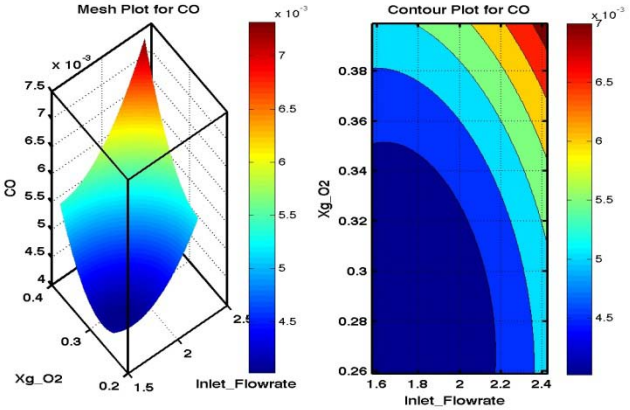
- Through developing advanced diagnostic tools to capture the data necessary for model development, verification and validation.



NETL's MFiX Solver

- NETL's open-source multiphase solver MFiX is used to perform basic and applied research to further the understanding and modeling of the many types of dense and dilute, reacting multiphase flows which are encountered in most advanced fossil energy technologies including gasification, coal combustion, gas cleanup and CO2 capture

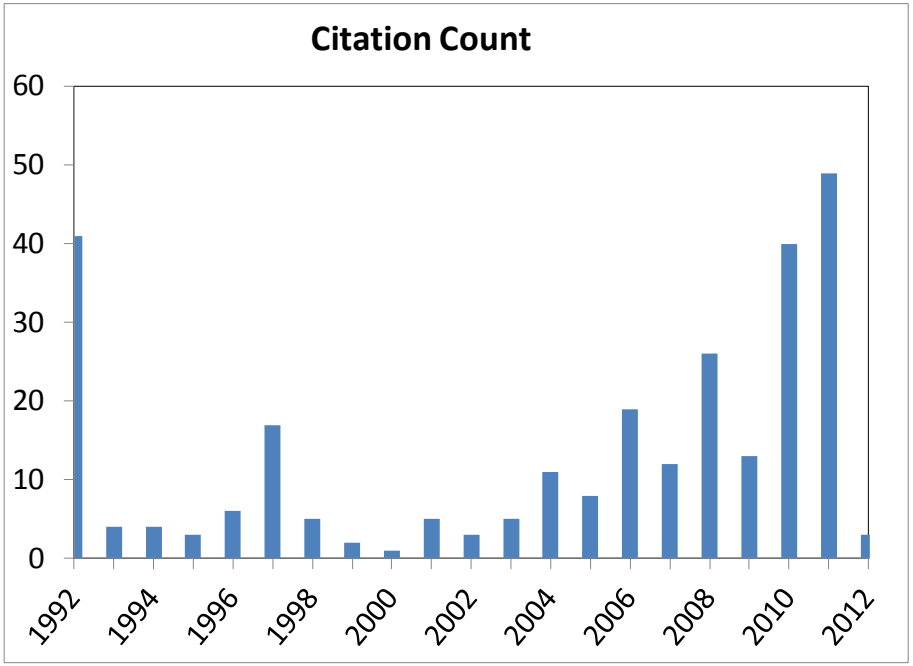
- MFiX suite of multiphase solvers such as MFIX-DEM, MFIX continuum, Hybrid MFIX and MFIX-PIC are being coupled with uncertainty quantification tool kit PSUADE from LLNL, to establish confidence levels associated with CFD simulations



- To accelerate time-to-solution, parallelization strategies such as hybrid MPI-OpenMP and GPGPU are being employed

MFIX Statistics

- **3050 registered users from 72 countries.**
- **The top 5 countries are:**
  - USA 830
  - China 517
  - India 284
  - Brazil 154
  - Germany 136
- **The 2012 sector breakdown is:**
  - Universities: 77%
  - Industry: 16%
  - National Laboratories: 8%
  - Others: 9%
- **Q1, 2013 sector breakdown is:**
  - Universities 73%
  - Industries 15%
  - National laboratories 2%
  - Others 9%



MFiX Multiphase Flow with Interphase eXchanges

http://mfix.netl.doe.gov

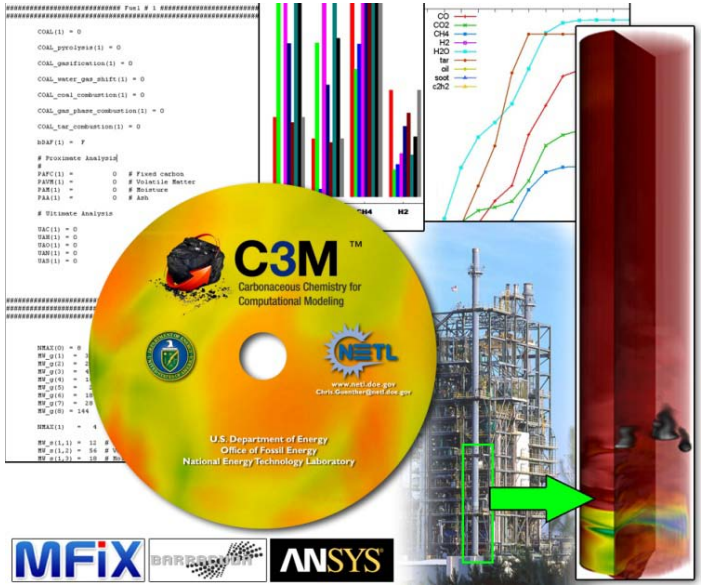
R&D 100

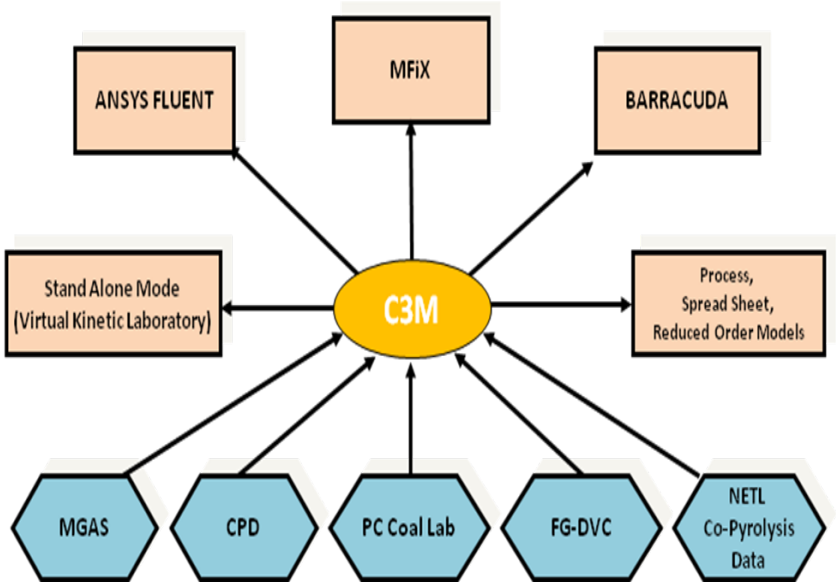
Future Direction of Multiphase Flow Science Team

- **Potential areas of interest to the RUA**
  - Development of three phase (gas/solid/liquid) capabilities in MFIX to enable the simulation of gas/liquid sorbent reactors
  - Development of high-fidelity, physics-based Reduced Order Models
  - Development of better sub-grid models, based on DEM simulations.
  - Implementation of higher order discretization schemes for two fluid model.
  - Development of non-Newtonian models in MFIX. With proper rheological models for slurry, sludge, blood etc.
  - Development of framework for Optimization under uncertainty with particular emphasis for multiphase flow applications
  - Development of a frictional stress model that is not as aggressive as the current models

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



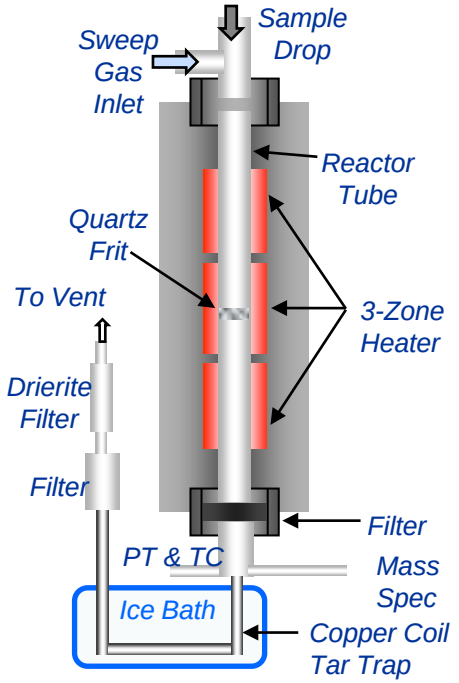


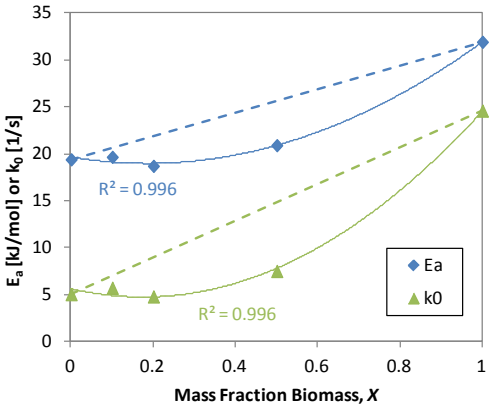
Why is C3M Needed?

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**

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**
- **Thermodynamic data**
- **Fuel Composition for CFD**
- **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**
- **Kinetic Data for Fuel Flexibility**
- **Easy, Intuitive, Reliable, and Graphical User Interface**

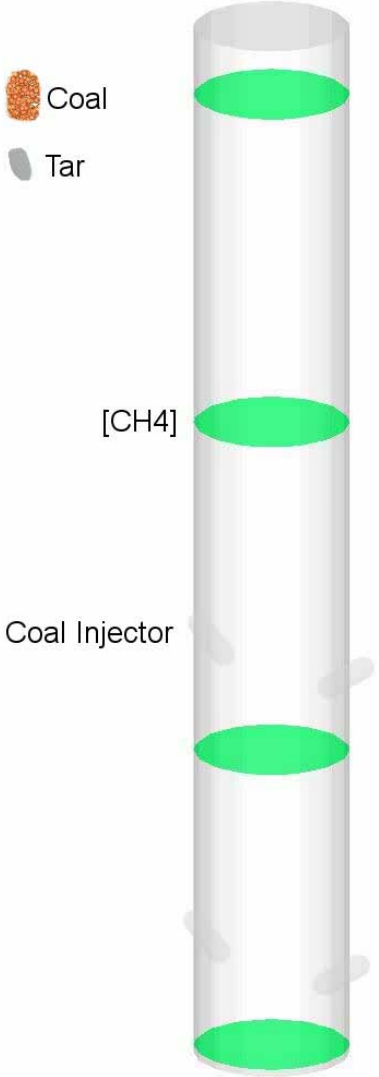




How is C3M Being Used in Industry?

Example: Transport Reactor Integrated Gasifier (TRIG)

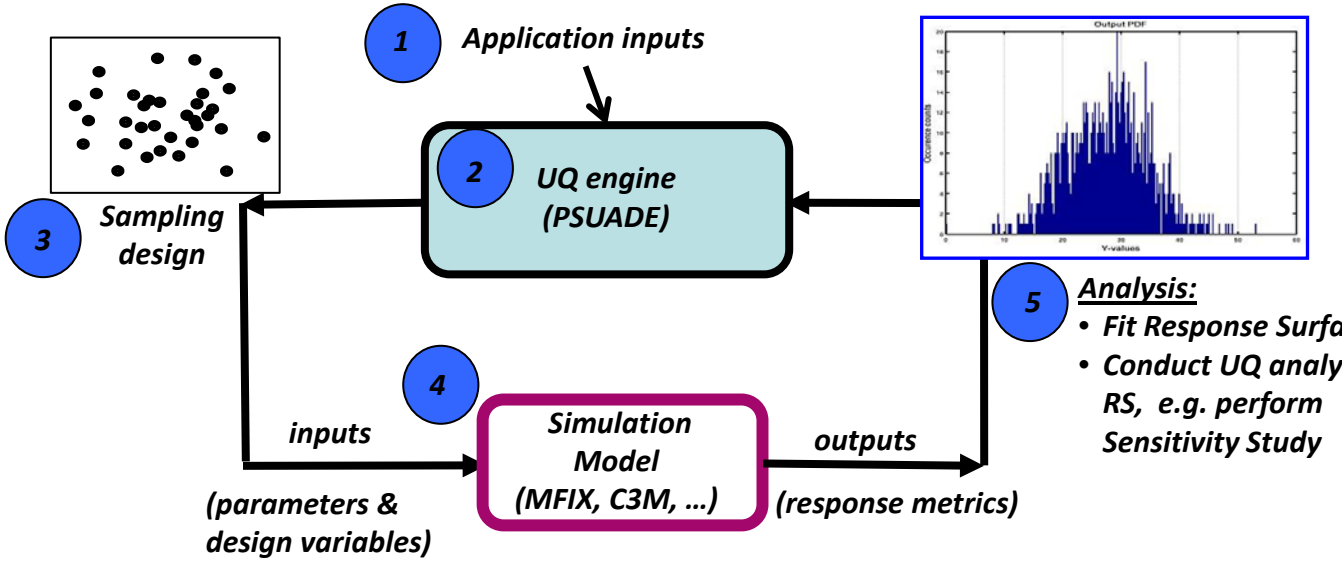
- **NETL and it's industrial partners are working together to commercialized TRIG technology**
- **C3M kinetics were applied MFiX and leading commercial codes FLUENT and Barracuda**
  - Establish state of the art in gasifier modeling
  - Evaluate pros and cons of each model
- **Helped refine design parameters and identify potential operational issues**
- **C3M allowed NETL to turn around a solution for the client in weeks rather than multiple months**
  - 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

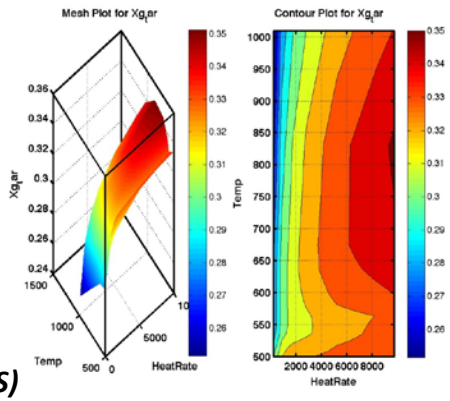
Uncertainty Quantification

Input Uncertainty Propagation and Quantification (Non-intrusive method)

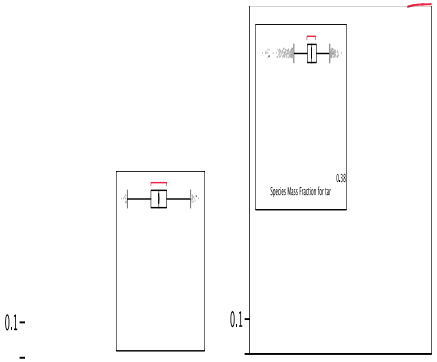


Analysis:

- *Fit Response Surface (RS)*
- *Conduct UQ analysis on RS, e.g. perform Sensitivity Study*



Response surface for tar pyrolysis process

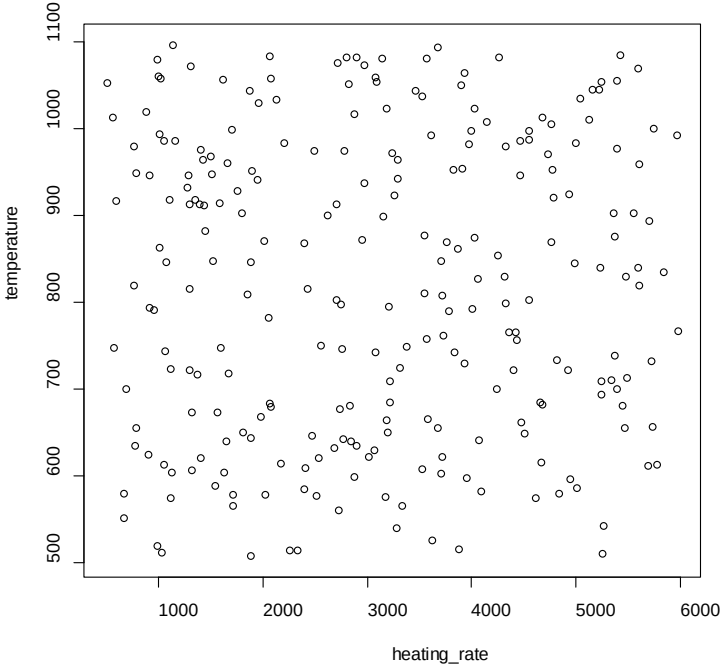


- ***No need to modify simulation models, treated as "black boxes"***
- ***No need for analysis of the mathematical structures in the model***
- ***May require large sample size for sufficient accuracy***

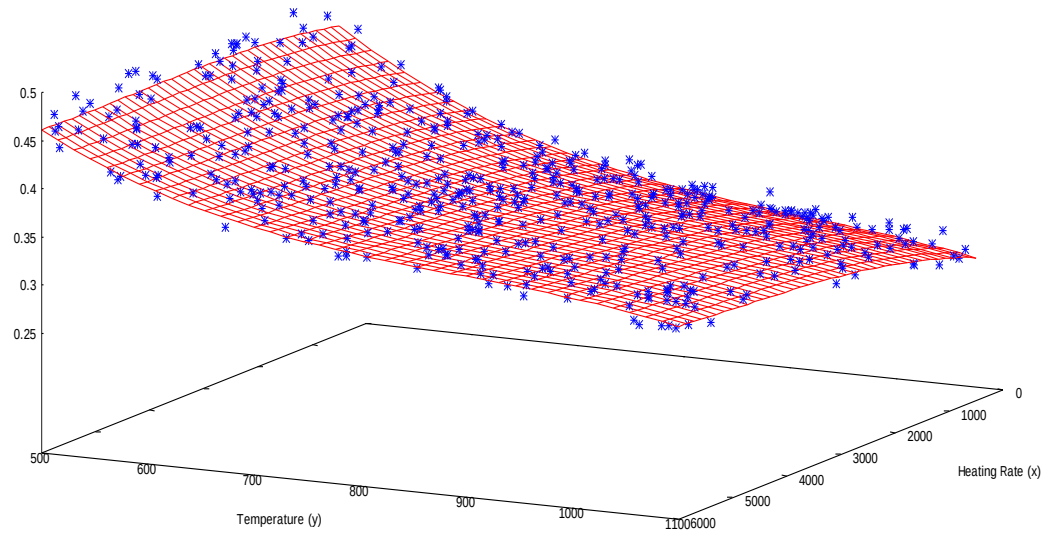
The Future of C3M

Response Surface Modeling in CFD

- **Simplify complex computational models for pyrolysis and gasification to simple algebraic expressions over wide operating conditions**
- **Format and output the algebraic expression into a form the CFD code can understand and use**
- **Improves CFD Fidelity without increasing computational cost**



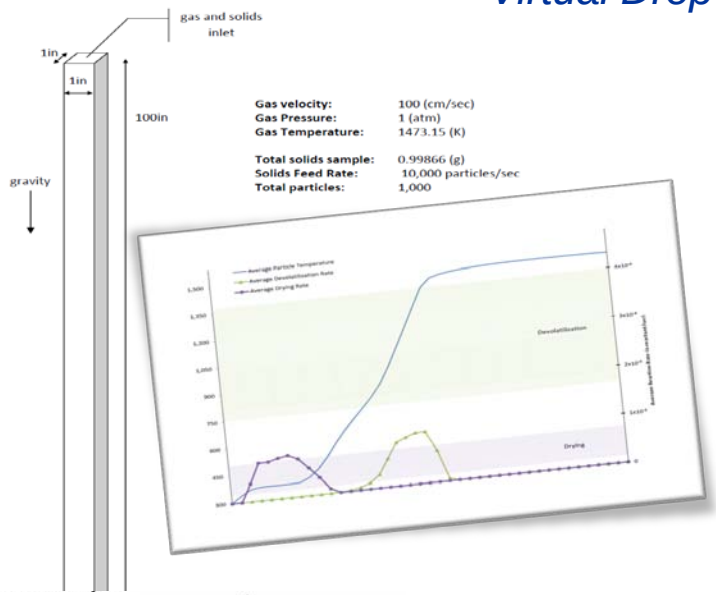
Design Space for PCCL

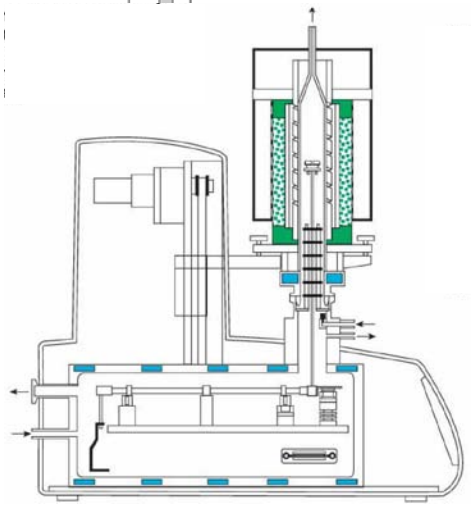


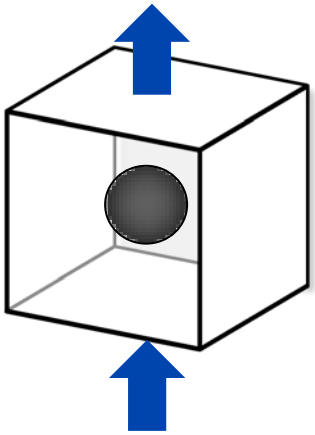
Example Response Surface
Tar Response to changes in Reactor Temp and Heating Rate

The Future of C3M

Virtual Drop Tube and Virtual HSTGA







- **Purpose:**
  - Provide a quick and easy test of global kinetic model within a simple CFD system
  - Evaluate realistic heating rates
  - Diagnose kinetic rates
  - Compare to common experimental data
  - Direct comparison to experimental weight loss curves and gas compositions
  - Great tool to refine kinetic models
- **Will be directly incorporated into the "Virtual Kinetic Laboratory" in C3M**

Role of NETL-RUA in C3M

- **C3M Development**
  - Richard Turton, Kiran Chaudhari (WVU)
    - Fundamental Code Development
    - Uncertainty Quantification
  - Sarma Pisupati (PSU, Energy Institute)
    - Gasification Equipment Development
    - Scale Validation
  - Nathan Wieland (WVU)
    - Fuel Flexible Reaction Rates
    - Gasification Dynamics