Radically Engineered Modular Systems (REMS):

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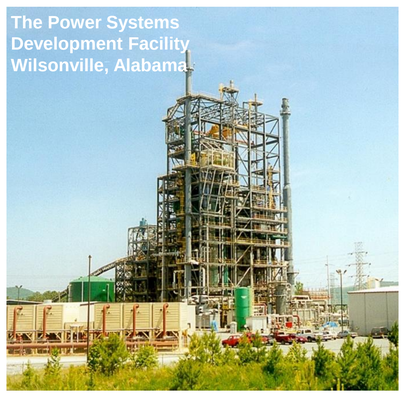
REMS Will Reduce Time, Cost, and Risk

Gasification Challenges:

- New approaches for coal to power/chemicals technologies $$$$ to develop & deploy
- Capital costs for plant ($$$$)
- Varying feedstocks, distributed power generation



How do we address?:

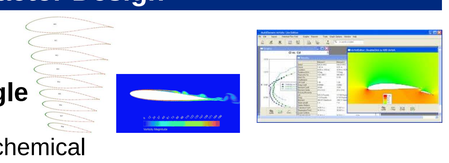
- Reduce time/risk scale up
- Reduce build/capital costs
- Fuel flexible designs, distributed systems
- Enhanced reactor/process performance
  - *Reaction manipulation at the particle level*

CFD led Reactor Design, Advanced Manufacturing, & Reaction Intensification offer unique opportunities to address these challenges

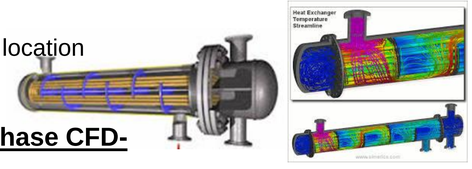
Radically Engineered Modular Systems (REMS)

Use CFD Simulation-Based Optimization for Reactor Design

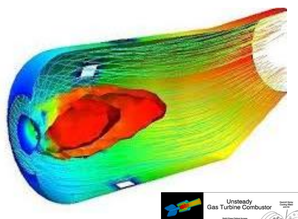
Build on Existing Techniques

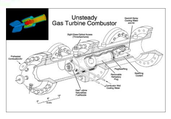


- **Use of CFD-Based Optimization is growing for single phase applications**
  - Proven technique in many engineering applications - chemical process, aerospace, turbomachinery, automotive
    - Optimization of airfoil shape for lift and drag
    - Optimization of heat exchanger tube shape, size, location
    - Optimal combustor design



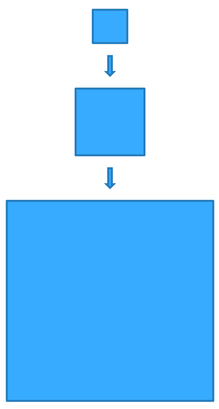
- **REMS will develop, validate, and apply a Multiphase CFD-based Optimization Toolset**
  - Multiphase CFD brings new challenges to the optimization process
    - Complex multiphase physics require accurate submodels for flow, heat transfer, chemical kinetics, coupling between phases
    - Very computationally intensive
    - Potential for huge datasets resulting from pilot and industrial scale applications
  - The new software capability will be based on the NETL **MFiX Suite** of multiphase flow CFD software





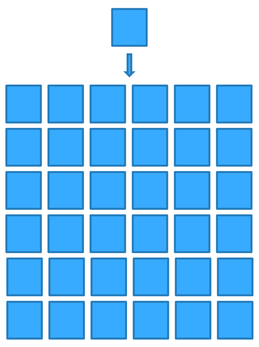
How Will REMS Differ from Traditional Approaches

Traditional



- Unreliable scale up
- Expensive, long development
- Incremental improvements

REMS



Beat economies-of-scale by using

- CFD to rapidly create novel reactor configurations
- Microwave, plasma etc. to intensify reactions
- Advanced manufacturing to replicate reactors at low cost

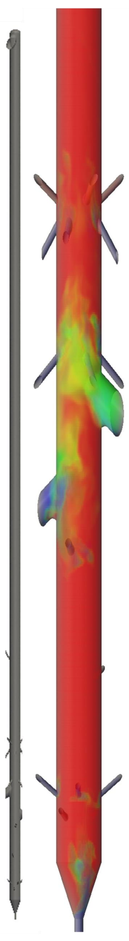
Example of Emerging Industrial Approach

Velocys: Small, Modular & Efficient GTL Reactors

Reactor Image from www.velocys.com

MFiX Multiphase Flow with Interphase eXchanges

Open source multiphase flow modeling for real-world applications



NETL's computational fluid dynamics (CFD) code, MFIX is central to the laboratory's multiphase flow reactor modeling efforts. This open-source software has over two decades of development history and more than 3,500 registered users worldwide. MFIX has become the standard for comparing, implementing, and evaluating multiphase flow constitutive models and has been applied to an extremely diverse range of multiphase flows applications. The successes achieved in modeling complex multiphase flow systems have led to new and improved key attributes such as drag, polydispersity, attrition, and agglomeration.

MFiX TFM is an Eulerian-Eulerian model which supports a broad range of capabilities for dense, reacting, multiphase flows by representing the fluid and solids as interpenetrating continua. This is the most mature MFIX model and is capable of modeling multiphase reactors ranging in size from benchtop to industry-scale. Approximation of the solid phase as a continuum typically allows for faster simulation time than Lagrangian techniques, however it also introduces the need for accurate mathematical models to capture realistic solids phase behavior. This includes transport properties, heterogeneous reaction kinetics, and constitutive relations for interaction between fluid and solid phases, e.g., solids phase drag and interphase heat transfer.

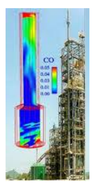
MFiX DEM is an Eulerian-Lagrangian model that treats the fluid phase as a continuum and models the individual particles of the solid phase. This is a relatively new variation on MFIX. While the treatment of individual particles can provide higher fidelity over a broad range of flow regimes (from dilute to packed), it also very challenging when dealing with very large numbers of particles for large-scale simulations. These large-scale applications will require high performance computing (HPC) resources and large amounts of computer time. Code optimization and speed up are critical research fronts to support industrial scale applications.

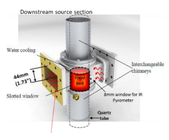
MFiX PIC is another Eulerian-Lagrangian model that represents the fluid as a continuum while using "parcels" to represent groups of real particles with similar physical characteristics. The MFIX-PIC approach offers reduced computational cost over MFIX-DEM as there are typically few parcels to track and parcel collisions are not resolved. However, the added modeling approximations impact the overall accuracy of the method. Development, validation, and optimization of modeling approximations are critical research fronts.

MFiX Hybrid is blend of MFIX-TFM and MFIX-DEM that represents the fluid as a continuum and models solids as either a continuous phase (TFM) or discrete particles (DEM). This technique is presently restricted to solving only the momentum equations to yield hydrodynamic predictions. This model is still in its infancy and has seen only limited testing.

ges from an MFIX-TFM simulation of a reacting transport gasifier colored by CO_2 mass fraction. Nearly million active grid cells used to capture the 100ft tall geometry. Momentum, thermal energy, and species mass conservations equations were solved for three distinct phases (two solids, and a gas mixture). ulation results provided by Tingwen Li, URS.

Radically Engineered Modular Systems (REMS): Research Areas





- **CFD-led reactor & process design (Bill Rodgers)**
  - Development of physics-based submodels
  - CFD Optimization and Toolsets
- **Reactor Characterization and CFD Model Validation (Ron Breault)**
  - 3D printing for rapid testing
  - Development of characterization tools
- **Advanced Manufacturing and Reactor Materials Development (James Bennett)**
  - Materials for unusual reactor geometries & conditions
  - Rapid, cheap, fabrication techniques
- **Reaction Intensification (Dushyant Shekhawat)**
  - Microwave/Plasma driven reactors
  - Catalyst Design

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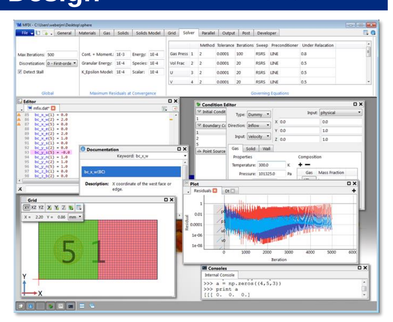
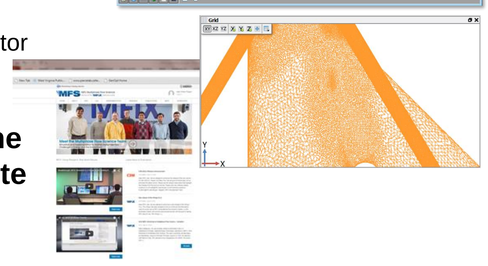
Use CFD Simulation-Based Optimization for Reactor Design

User Interface and Toolset to Manage the Optimization Process

- **Design and develop GUI-based, Multi-objective Optimization software framework**
  - Code infrastructure for managing the optimization process
  - methodologies and code to create and manage reactor models created using MFIX Suite of multiphase flow software
- **The modeling tools will become part of the publicly available, Open Source MFIX Suite of codes (https://mfix.netl.doe.gov)**