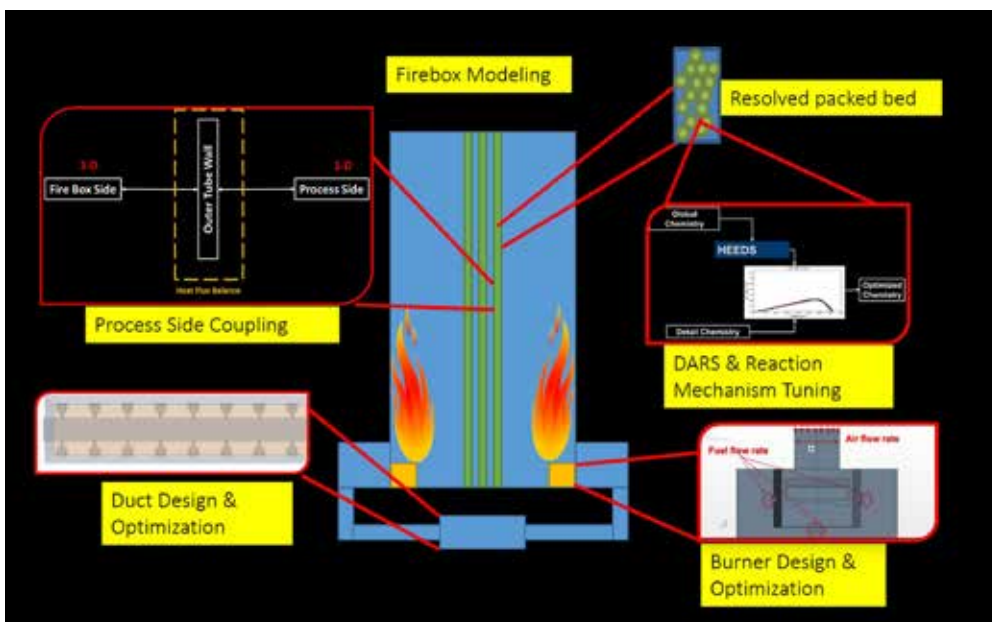# Multi-scale modeling of furnaces and reformers

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Figure 1: Various design considerations in a reformer

The design of furnaces, process heaters, crackers, and reformers is very challenging. This is due to the high temperature environment and complex chemical reactions occurring at various spatial and temporal scales. Optimum design and operation needs to balance thermal, environmental and process performance simultaneously. Furnace and cracker operations involve the processing of large volumes of feedstock, and even small improvements in equipment and process efficiency can translate into improved operational efficiency and significant cost savings. Computational fluid dynamics (CFD) can help in the design and operation of plants and processes to achieve these goals.

Heaters and reformers have two major components: the firebox where combustion is occurring and the process side tubes where the feed is being converted to
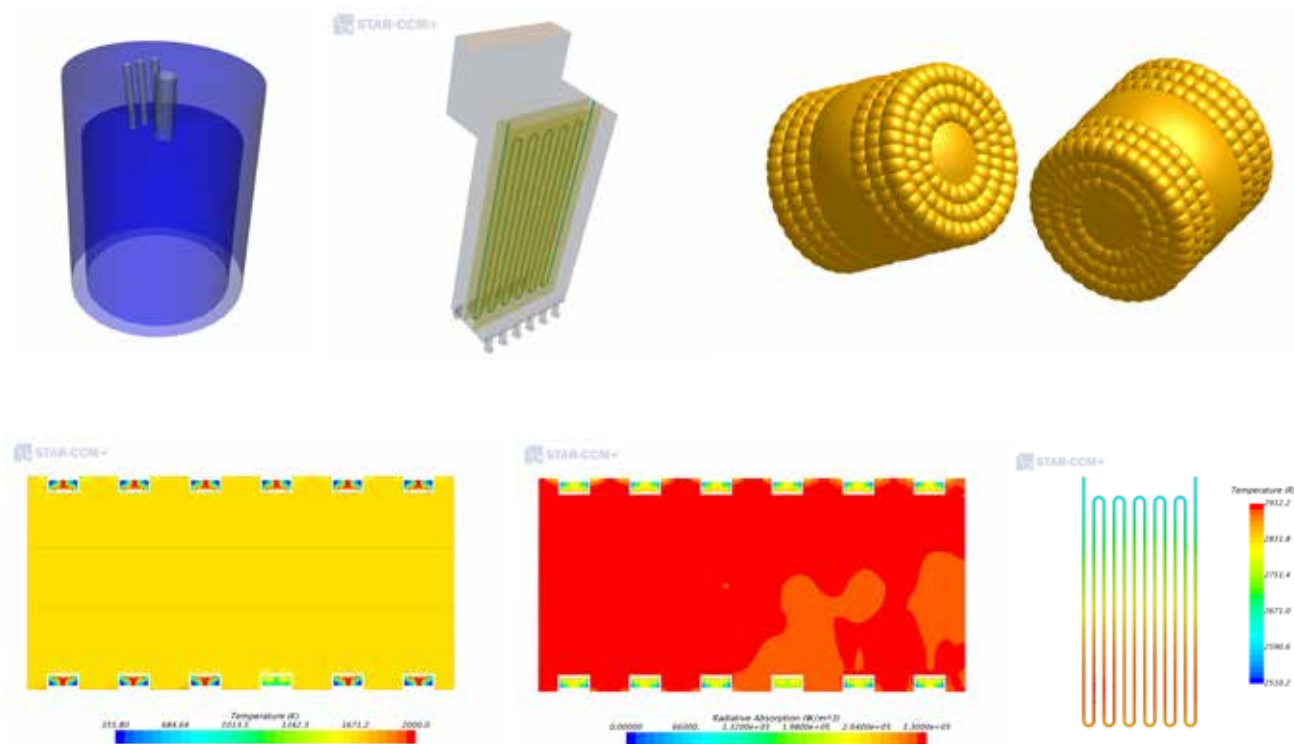
Figure 2: Burner range of geometric scales and mesh (from 0.005m to 15m) (top)

Figure 3 : Temperature distribution and radiative absorption in the burner (below)

products. The design challenge arises due to the functioning of multiple components: multiple burners in the firebox side, multiple tubes in the process side, catalytic reactions, and thermal processes inside the coils. The performance considerations in CFD-based design include efficiency, emission control, and uniform heat distribution and conversion rate in the processes.
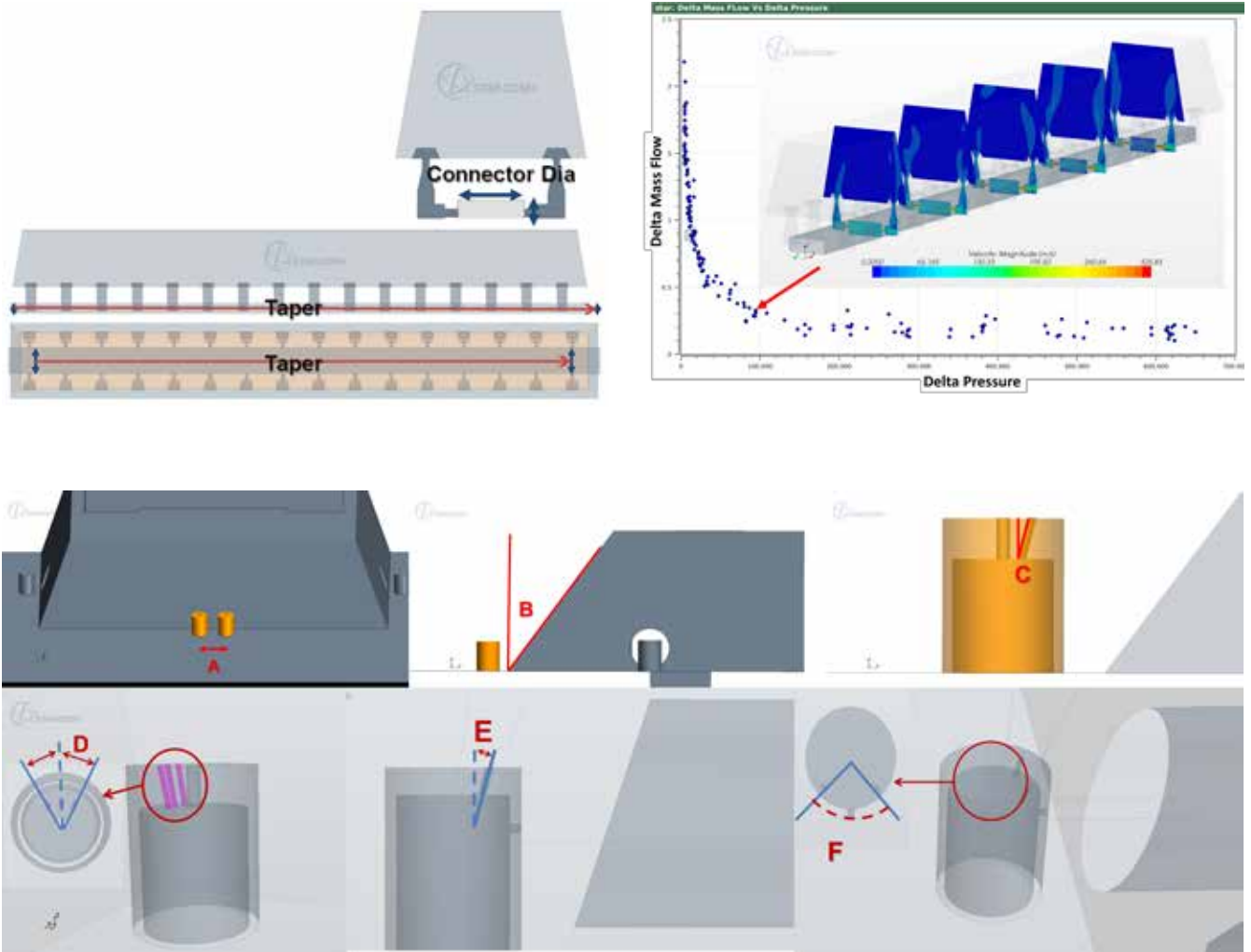
In this article, we explore the application of CFD to various components of furnace and reformer design using a hierarchical approach. These hierarchical scales of processes (a combination of geometrical and physics scales) are shown in figure 1. Overall, one can classify them as:

Macro Scale Models	Meso Scale Models	Micro Scale Models
Firebox combustion modeling for thermal performance	Catalyst shape and packed bed modeling for yield	Reaction kinetics and reaction mechanism tuning
Burner design and optimization for flame shape and pollutants	Coupling to reaction kinetics on process side for thermal performance	
Air supply duct optimization of uniformity of airflow		

Firebox modeling

The firebox houses the burner and requires uniform fluid flow and heat distribution to achieve good operating efficiency. Figure 2 shows a typical burner with geometric scales ranging from 0.0016m to 25m, a factor of 15,000. The first modeling challenge in such a geometry with wide ranging scales is to create a high quality mesh that takes a short amount of time to generate. A good mesh should have refinement to capture the small geometric details but be coarse enough to keep computational times reasonable. The meshing capability of STAR-CCM+® Software (polyhedral or trim depending on the need) and automated prism layer meshing ensures that the burner geometry can be easily meshed. The automatic meshing capability which allows customization of refinement regions ensures such a mesh can be created with little manual input. Qualitative and quantitative burner performance characteristics can be assessed from the results, allowing the designer to analyze oxygen concentration, temperature uniformity, recirculation zones, and flue gas engulfment. Further, the radiative and convective heat transfer duty of the tubes can be evaluated as well. Poor temperature uniformity can lead to high temperatures on the tubes, in turn leading to excessive coking and poor performance of the heater, requiring an earlier than scheduled downtime. A full suite of combustion models, multi-component species modeling and radiation modeling allow for all the physics to be accounted for. Figure 3 shows

sample results from STAR-CCM+ showing the temperature distribution and radiative absorption in the burner and heating tubes.

Heater duct optimization

The next step is to design the heater ducting with minimal mass flow variation through the burner throats and minimal pressure drop. A properly optimized heater duct design (using STAR-CCM+) shortens the product development cycle and reduces the risk of poor performance. The heater consists of a central duct connected to the burners via short legs. For this example, the radius of the connector, width and height of ducts were chosen as the design parameters (figure 4) for optimization analysis.

The heater performance was simulated in STAR-CCM+ and design optimization was conducted with HEEDS™ software, driven by the hybrid adaptive SHERPA algorithm. HEEDS drove the parametric CAD geometry and STAR-CCM+, performing 148 design evaluations by varying the design parameters. The baseline design analysis

took 40 minutes on eight cores and the entire design optimization was performed in 32 hours on 40 cores. Siemens PLM's Power Token licensing provided complete flexibility to use the most efficient combination of parallel evaluations and solver cores for the problem at hand. Mass flow and pressure changes were used as benchmarks for the best design. Figure 5 shows the results from HEEDS evaluations, showing the design with the optimum combination of mass flow change and pressure change within the heater. Thus, STAR-CCM+ and HEEDS optimized the heater duct design within a few days, saving valuable time and cost and reducing the number of prototypes and testing while improving performance.

Process burner optimization

Burner design can affect the flame shape and length, which in turn changes the temperature distribution in the furnace. The resulting heat density effect alters the flue gas recirculation patterns. In low NOx burners, this will also change the NOx emission levels. As such, an optimized

Figure 4: Design parameters for heater duct optimization analysis (top left)

Figure 5: HEEDS results showing best combination of mass flow and pressure drop in the heater (top right)

Figure 6: Process burner design parameters for optimization in STAR-CCM+ (below)
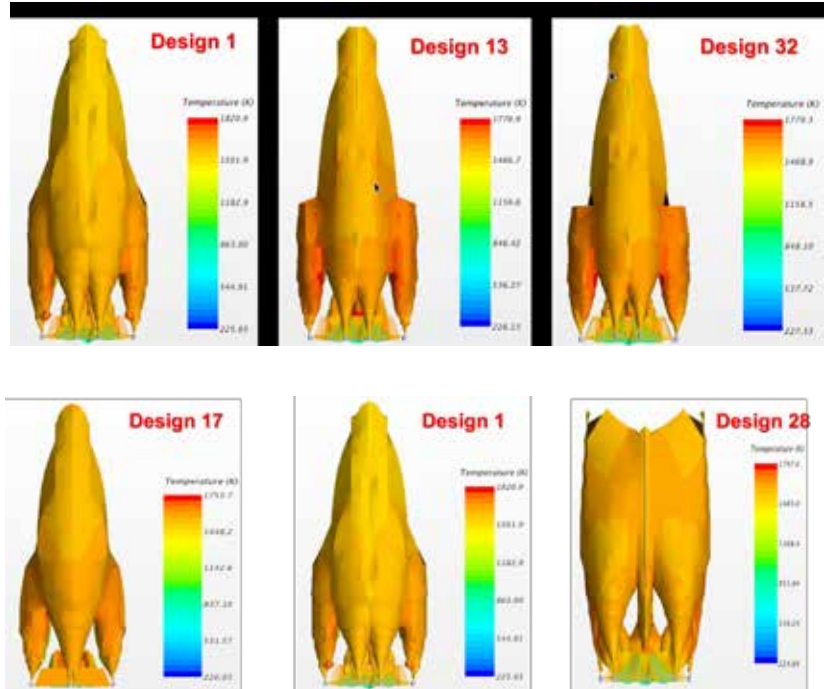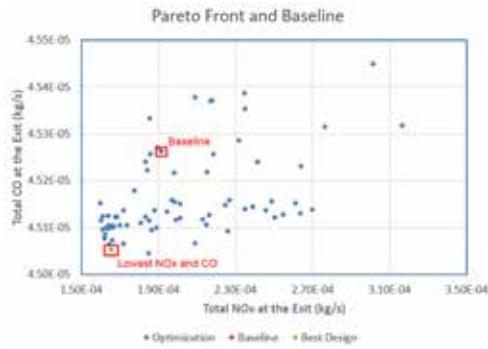
Figure 7: Pareto front and comparison of flame height for baseline and best designs for tilt angle changes (top)
Figure 8: Flame comparison between baseline and best designs for different injector spacing (below)

burner design is critical to maintain peak furnace performance from both thermal and environmental perspectives. Here, a full design optimization of a single flat flame burner using STAR-CCM+ and Optimate+, a plugin that utilizes the SHERPA search algorithm of HEEDS, is described. The design objective is to reduce the CO and NOx relative to the baseline design. The dependence of the flame height and emissions on burner design parameters like tilt angle and fuel port spacing is explored. A fully optimized burner design should have good flame stability, an acceptable flame pattern, length/shape, no flame impingement or flame to flame interaction, good combustion efficiency, and meet stringent emission standards.

The burner has four fuel ports with fuel and oxidizer entering at standard temperature and pressure. The burner heat release is approximately 0.9MW. Figure 6 shows the six design parameters used in the study. The simulations were run with the K-Omega SST turbulence model, the Presumed Probability Density Function (PPDF) equilibrium combustion model, NOx PPDF flamelet and the Discrete Ordinates Radiation Model.

Design constraints were built into the model to not exceed a volume average temperature greater than 1350°K in the firebox and a flame height larger than approximately 1.7m based on process heating needs and design of the furnace. Optimate+ automatically varies the design parameters and a total of 85 design evaluations were run; 13 designs did not meet the constraints and were rejected. The best performing design (figure 7) minimized the CO by 4.5 percent and NOx by 13 percent compared to the baseline results. This design had a tilt angle of 16 degrees compared to a tilt angle of 1 degree for the baseline case. The design also showed a 3 percent flame height reduction. A design with a tilt angle of 24 degrees (Design 32) showed lesser CO and NOx variation but with similar flame height. Table 1 shows a comparison of the baseline case with the best designs from Optimate+.

The influence of fuel injector spacing was also investigated in the optimization analysis. The baseline design had a spacing of 88mm and the best performing designs had a spacing of 25mm (Design 17) and 250mm (Design 28) respectively. Figure 8 shows the comparison of flame

Table 1: Comparison of baseline and best designs

	Design 1	Design 13	Design 32
Flame Height (m)	2.423	2.342	2.422
Flame Volume (m3)	2.15E-01	1.86E-01	1.84E-01
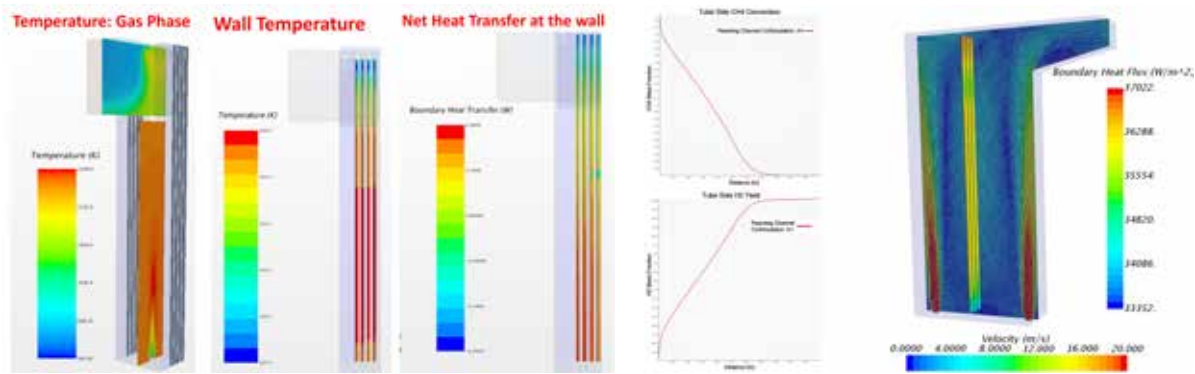
height and volume for these designs. A 5 percent reduction in CO and 3.4 percent reduction in NOx was achieved for Design 28 but the flame height reduced by 28 percent.

The design optimization study from changes in tilt angle and injector spacing showed that Design 32 was the best design overall, showing a 4 percent CO reduction and 11 percent NOx reduction from the baseline cases.

Reacting channel co-simulation

The next component in the furnace design optimization is the process tubes in the reformer. Full 3D modeling of the process side with tubes is computationally expensive since there are multiple burners (firebox side) and tubes (process side). A computationally efficient method is co-simulation in STAR-CCM+, with 3D modeling of the firebox side coupled with 1D modeling of the process side.

The firebox side is modeled in 3D with turbulent flow, fuel/oxidizer boundary conditions, combustion models and participating media radiation model, accounting for full heat transfer. On the process side, any number of tubes can be accommodated and the tube is modeled as a 1D plug flow reactor (PFR), along with complex tube side reactions and heat exchange between firebox and process side. No meshing is needed for the 1D model saving valuable computational time. For the coupling, temperature is provided to the process side from 3D simulations and heat flux is provided to the firebox side from 1D analysis.

Figure 9 shows a sample output from co-simulation showing temperatures on the firebox side. For kinetics of process side reactions, detailed, reduced, or user-defined mechanisms can be used.

Packed bed heat transfer modeling

The design of a packed bed reactor should consider the influence of packing geometry on fluid flow, heat transfer, and pressure drop. This requires a reasonable amount of experimental trial and error to investigate kinetics, heat transfer, and fluid flow behavior to confirm a final reliable design. With the Discrete Element Modeling (DEM) capability in STAR-CCM+, industrial scale simulation of packed beds is now possible by fully resolving the geometry of the beds, enabling reliable parametric analysis for reactor design and providing detailed insight into physics like local velocity and recirculation.

Generating a representative bed could be done manually, with the Monte-Carlo method or with a scan of the bed. All these methods are time consuming and expensive. With STAR-CCM+, the packing can be generated in a fast, physics-based and cost-efficient way using DEM. A completely automated workflow for packed bed simulation is possible, incorporating DEM, CFD and automation.

Figure 11 shows porosity values of non-spherical packings compared to experimental data for packings of spheres, cylinders, and cylinders with holes. DEM spheres are clustered to form a single element. Generation of the random packing is done with DEM and the positions of individual elements are fixed and exported. The geometry of the packed bed is created from the position and automated polyhedral meshing with proper contact resolution generates the computational mesh.

The simulation was run in STAR-CCM+ at a Reynolds Number of 6804 and wall temperature of 100°C. A sample comparison of heat transfer and porosity between STAR-CCM+ and experimental

Figure 9: STAR-CCM+ results from Co-simulation in firebox side
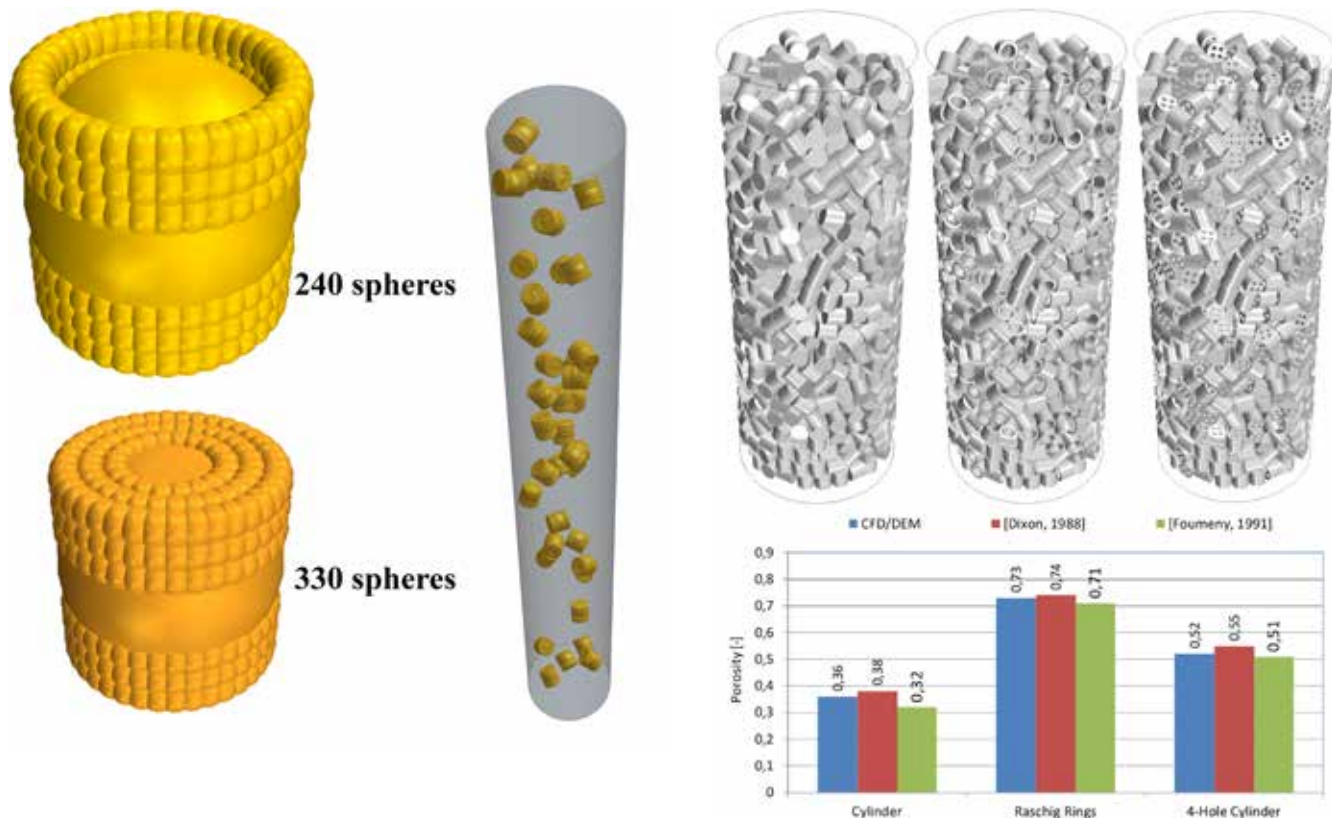Figure 10: Process side results showing temperature, heat flux and species conversions

240 spheres

330 spheres

data for the packed bed is shown in figure 12. STAR-CCM+ accurately predicts the packed bed physics (porosity, flow field and heat transfer) and enables reliable parameter design and optimization.
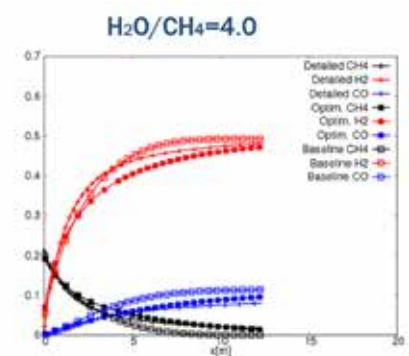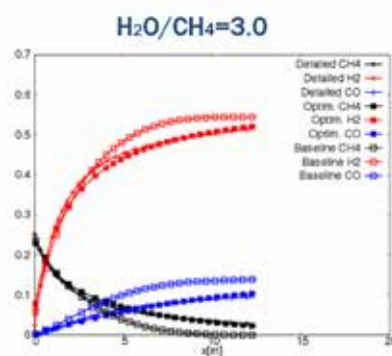
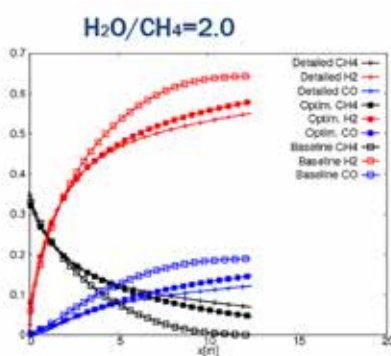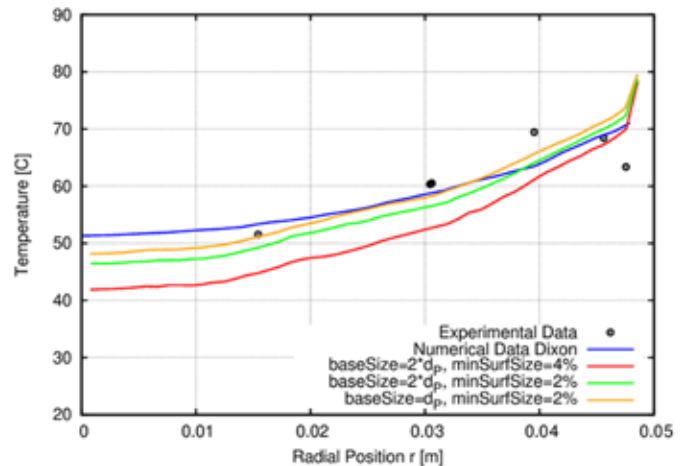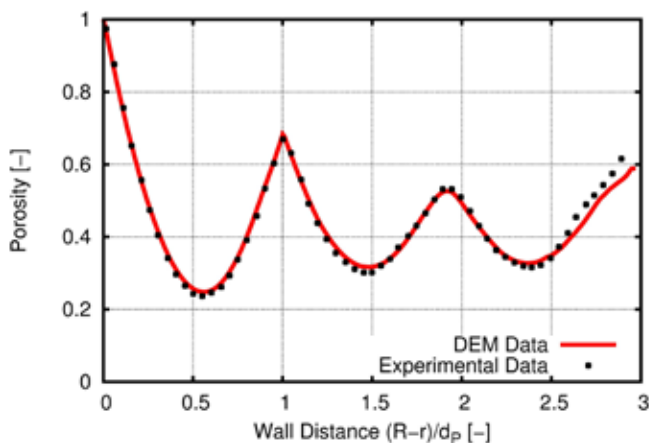**Reaction mechanism optimization**

The final part of the design puzzle is tuning the chemical reactions in the reactor. DARS (Digital Analysis of Reacting Systems) is a tool within STAR-CCM+ for 0D and 1D management and analyses of chemical reactions and modeling ideal reactors. Together with HEEDS, a global kinetic mechanism consisting of only a few reactions can be tuned to reproduce the results from a detailed (and accurate) reaction mechanism

the accuracy of a detailed reaction mechanism. With DARS and HEEDS, an optimized global mechanism can be developed in simple canonical systems that can be used in STAR-CCM+ at a computationally lower cost. A 12.5m packed bed reactor was analyzed with DARS at several H_2O/CH_4 ratios. Detailed and global chemistries are outlined in table 2. CO, H2, CH4 and temperature axial profiles are then transferred to HEEDS. The design objective in HEEDS is to minimize the root mean square (RMS) between the detailed chemistry reference curves and the global chemistry results. The chemistry parameters, pre-exponential factors, and activation energies were modified within the specified range by HEEDS and the DARS simulations

	Detailed Chemistry [1]	Global Chemistry [2]
Number of species	8 gaseous/13 Surface	5 species
Reactions	42 reactions	$CH_4 + H_2O = CO = 3H_2$ $CO + H_2O = CO_2 + H_2$ $CH_4 + 2H_2O = CO_2 = 4H_2$

before being used in STAR-CCM+ simulation. Since detailed reaction mechanisms in CFD are computationally expensive, this method can reduce the computational burden yet assure

were run again. A total of 1,000 reaction designs were analyzed by HEEDS within two hours. A comparison of the baseline, detailed, and best designs are shown in figure 13. The

optimized reaction mechanisms were then used in the CFD simulations in place of the detailed chemistry, significantly reducing the computational cost with this automated workflow.

Conclusion

With CFD, a true data driven decision-making process while exploring design alternatives is possible for the design of reformers, heaters and furnaces. The combination of STAR-CCM+, DARS and HEEDS allows chemical engineers to simulate and optimize the performance and design of such equipment at the system and unit level. This multi-scale, multi-physics coupling approach can alleviate operational performance concerns while delivering improved reformer designs at reduced time and cost.

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Figure 12: Comparison of heat transfer and radial porosity (top)
Figure 13: Comparison of baseline, detailed, and optimized reaction chemistry (below)