This white paper explores the role of computational fluid dynamics (CFD) within the realm of chemical reaction engineering. The initial goal is to understand how using STAR-CCM+® software for CFD simulation to analyze and optimize chemical reactions enables you to improve reactor designs. We will investigate transport processes in various reactor types, providing information on how to explore alternatives to model better reactor designs in less time. By creating the best design possible, you can positively influence production efficiency while lowering costs.
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Executive summary

Chemical reaction engineering specifically deals with chemical reactors. It is also referred to as reaction and/or reactor engineering. The primary goal of chemical reaction engineering is to optimize transport processes, such as heat transfer, mass transfer and mixing, to improve product yield/conversion and reactor operation safety. Simply said, it helps maximize yield while minimizing costs, such as those associated with feedstock, energy input, heat removal or cooling, stirring or agitation, pumping to increase pressure and/or frictional pressure loss.

From the standpoint of CFD, reaction engineering is the application of transport phenomenon and chemical kinetics knowledge to industrial systems. Transport phenomenon is key and defines which property is important. Chemical kinetics, or the study of rates of chemical processes, is founded on the experimental study of how different conditions influence the speed of a chemical reaction and its mechanism and transition states; and on the development of mathematical models representing the reaction’s characteristics. Essential aspects of a chemical reactor design are shown in figure 1.

Figure 1: Essential aspects of chemical reactor design.
Reactor design and CFD

Designing a reactor involves a number of key considerations, including:

- Reactants/products phase or state comprising solid, gas, liquid or aqueous/dissolved in water
- Reaction type, including single, multiple and parallel series or polymerization
- Catalyst identification, which may take in flow distribution and mixing
- Species transport
- Operation mode, such as batch, semi-batch or continuous

Considering underlying transport processes, such as fluid flow, heat transfer, mass transfer and reactions, is beneficial as CFD simulation can add substantial value to these characteristics.

There are many steps in a reactor design process that enable you to take the discovery of a new chemical with novel properties from concept to commercial production, including:

- Conceptualizing how you analyze new chemistry and develop a business case
- Lab scale to accommodate analysis of kinetics, catalysis, thermodynamics, material properties and toxicity
- Reactor selection involving the analysis of flow regime, heat release, residence time distribution (RTD), liquid hourly space velocity (LHSV) as well as gas hourly space velocity (GHSV)
- Engineering with idealized models for analysis of plug flow or continuously-stirred tank reactors (CSTR), volume sizing and overall heat transfer
- Preliminary design of vessel configuration, internals, baffles and coils
- Scaleup simulations, including pilot scale design, scaleup parameters and design space exploration
- Final design to encompass the extrapolation from scaleup rules, flow modeling, safety, risk and runaway reaction analysis and dynamic modeling
- Commercializing with startup, troubleshooting and operator training

You can use an idealized reactor model that has been sized to lab or bench scale to initiate the engineering process and predict key reactor behavior variables, including reaction parameters, material properties, toxicity, ideal operating conditions, optimal catalysts and preliminary reactor dimensions.

The next step is to establish a preliminary reactor configuration followed by the escalation and simulation of a pilot-scale design. Finding the sweet spot for a pilot-scale design is typically the greatest challenge, as nonlinear-linked parameters can cause each subprocess to scale differently. If you want a larger capacity, geometrically increasing the size is sufficient; but that does not work for reaction, heat transfer or mixing processes. Sizing the model based on turbulence scales may result in extremely high revolutions per minute (RPM) or a design that is geometrically unfeasible. While you can use various scaleup results to create many different designs, design space exploration is required to find ideal conclusions.

You can achieve a final proposed design by using the scaleup rules, detailed flow modeling, safety and runaway reaction assessments along with dynamic system modeling. The resulting data will help you predict how the design will work at plant scale. Figure 2 walks you through reactor design and scaleup phases and shows how CFD can help you better predict the overall capability, fidelity and efficiency of your final design.

Figure 2: Standard reactor design and scaleup phases in which CFD can add value.
Supporting software solutions for reaction models

Commercial software solutions can assist you in understanding various multiphysics reaction scenarios. For example, a wide range of chemical reaction models and solving capabilities are available in STAR-CCM+, including models for the:

- **Gas phase**: Simple combustion reactions or reactions that take place inside tubes such as those in cracker furnaces with external heat supplies
- **Liquid phase**: Polymerization schemes or series-parallel liquid reactions with meso/micro-mixing
- **Custom reactions**: Enzymatic reactions, fermentation and user coding

In addition, STAR-CCM+ includes the Digital Analysis of Reacting Systems (DARS) module for the management and analysis of complex chemical reactions that involve detailed chemical kinetics.
Gas-phase-reacting flow models

The most basic types of flow models are for gas phase reacting flows in which different species (feedstocks) enter the reactor non-premixed, completely mixed or partly premixed. For each category, various STAR-CCM+ models are available to help you simulate the reaction (see table 1).

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<th>Conceptualization</th>
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Some models are regarded as tabulated chemistry models to reduce computation times, while others make use of detailed chemistry in DARS. A simple glass furnace is a representative example in which air and fuel that is not premixed enters the domain. The simplest model is an eddy break-up (EBU) combustion model that is referenced in figure 3, which highlights the flame zone and the region of NOx formation within the overall combustion chamber. NOx is a generic term for mono-nitrogen oxides NO (nitric oxide) and NO2 (nitrogen dioxide).

In this case, critical considerations for design and reactor operation include heat transfer as well as pollutant-species production, such as NOx.

Validation studies conducted for the gas-phase-reactor design are summarized in figure 3. The top plot shows the temperature profile at a location approximately 0.9 meters downstream from the fuel inlet. The green dots show experimental measurements, and the blue line indicates STAR-CCM+ simulation results. As the plot shows acceptable agreement between the two sets of data, you can confidently predict the safe operation of this type of reactor.

Also important is species concentration, such as oxygen (O2) mole fraction at the same location, which is shown 0.9 meters from the fuel inlet. The bottom plot in figure 3 validates agreement between experimental measurements and simulation results. In situations in which high-temperature processes make experimental work difficult and expensive, simulation provides an easier, more cost-effective way to explore targeted quantities.

Table 1: Reaction models for gas-phase-reaction flow in STAR-CCM+.
Figure 3: Eddy break-up model of glass furnace highlighting flame zone and NOx region in the combustion chamber.
Modeling process for heaters and crackers

In process heaters and naphtha crackers, reactants pass through a tube while heat is supplied by combustion outside the tube. By using STAR-CCM+, you can provide a simplified way to simulate these reactions by modeling the tubes as one-dimensional (1D) plug flow reactors, an idealized model option used to describe chemical reactions in continuous, flowing systems of cylindrical geometry, while the external combustion is modeled in 3D. This approach is much less computationally expensive than simulating the whole system in 3D.

Conduction, convection and radiation are modeled in 3D on the outer tube wall, and heat transfer via convection is modeled in 1D. The two simulations are coupled at the tube wall junction. This process allows you to explore how mass fractions of species behave inside the tubes and simultaneously look at heat transfer and temperature profiles outside the furnace tubes. Figure 4 shows the results for a coupled 1D/3D simulation of a steam methane reformer, providing the axial distribution of temperature, heat flux and species concentration.
Detailed chemical kinetics

Figure 5: Flamelet libraries and lookup tables for gas and surface chemistry simulation.

DARS is for standalone, gas-phase-detailed chemical kinetics and can be used for simulating ideal, or simplified, reactor models. By using the DARS module, you can develop and import reaction mechanisms to perform sensitivity analysis, validating experimental data and simplifying the reaction mechanisms in your CFD simulations. Figure 5 shows the DARS gas and surface chemistry graphical user interface (GUI) along with flamelet libraries and lookup tables for gas and surface chemistry simulation.
Surface chemistry formulation

Surface chemistry is an important class of detailed simulation and represents scenarios in which the reactants are initially adsorbed onto a surface medium that acts as a reaction catalyst. Once the reaction is completed, the products are desorbed, or released, and the surface is left unchanged. You can model surface chemistry either with detailed chemistry formulations using the stiff differential equation solver in STAR-CCM+, or by using global reaction mechanisms.

An important application of surface chemistry involves designing packed-bed reactors, which consist of tubes filled with a packing material impregnated with catalysts to improve contact between two phases in the reaction. Design challenges include accurate prediction of heat transfer, which is critical for safe reactor operation. Modeling these types of reactors provides critical insight into heat transfer generation that is representative of randomly-packed beds, and resolving contact while meshing can be done efficiently and accurately.

By using STAR-CCM+, you have an automated way to model and simulate packed-bed reactors. Through a user-friendly GUI, you can specify geometry conditions, particle properties, wall properties, particle-to-particle interactions as well as other fluid properties, and heat transfer simulations. Once these specifications are defined, you can generate the catalyst bed using the built-in discrete element modeling capability in STAR-CCM+. The software allows you to create a mesh, including boundary layers, and perform CFD simulation; and you can use postprocessing to look at radial and axial porosity, velocity profiles, heat transfer and reactions as required.

Figure 6: Automated process to simulate packed-bed reactors.
Using CFD simulation to perform and validate lab scale tests is essential to the scaleup operation. The validation process can help you gain confidence in model robustness and fidelity, and enable you to make predictions at plant scales when it may not be possible to take measurements. In one example, we looked at determining the power calculation for a variety of solids with concentration levels of 10, 20, 30 and 40 percent by weight. A four-bladed pitched bladed turbine (4PBT), which is shown in figure 7, was used to suspend sand with a particle size of 190 particle size microns in water at a speed of 600 RPM. The liquid and solid densities were 1,000 and 2,483 kg/m$^3$ respectively. The tank had a height and diameter of 0.34 meters with an impeller diameter of 0.19 meters. Figure 8 shows STAR-CCM+ simulation predictions that accurately validate power consumption data and predict a sub-parity in the power increase. Documented predictive power correlation charts should be used to match/confirm system condition(s) for geometric ratios, material properties and solid concentrations.

Based on case-specific geometries and material properties for a designated factor, often it is impossible to find an appropriate match for a given design requirement; and, as a result, the designer’s confidence to choose the right power number may be adversely affected. This uncertainty results in inaccurate power predictions from correlation-based methods as reflected in the plot shown in figure 9.

Figure 7: Lab scale mixing vessel used in solids suspension experiments.

Figure 8: Power consumption comparisons: Contour plots show the volume fraction for the various solid loadings.
Liquid-phase reactions

Liquid-phase reactions significantly differ from gas-phase reactions because the liquid's rate of diffusion is much lower than its viscosity; therefore, liquid-phase reactions can be strongly influenced by scalar gradients. The most important difference in this scenario is the phenomenon of micro-mixing, or mixing at the molecular scale. In figure 9, the reactor’s physical configuration will determine whether the reaction will preferentially form product S or, alternatively, product R. In this schematic, for example, the location at which species B is added, either at the vessel’s top or close to the impeller, can significantly alter the results.

Figure 9: Physical reactor configurations essential in predicting liquid phase micro-mixing reactions.

Figure 10: STAR-CCM+ allows you to accurately model and predict micro-mixing effects by providing the eddy contact micro-mixing model, which results in higher accuracy compared to the EBU model (which is typically used for gas-phase reactions). The eddy contact model helps you calculate a reaction time scale based on scalar dissipation rate, which is used to calculate the reaction rate.
Customized reaction models: fermentation and biochemical reactions

Another type of flow reaction consists of fermentation and biochemical reactions in which sugar is converted to acid and produces either gases or alcohol through a complex chemical reaction. Differing reaction rates occur starting with a log phase to exponential and deceleration phases and ending with a stationary phase. Each phase has its own defined reaction rate. You can define each of these rates using the custom-reaction definitions available through the user-defined or field functions in STAR-CCM+.

![Diagram of reactor models](image)

- **Packed-bed reactors**
  - DEM backed mesh
  - Dedicated GUI

- **Fluidized bed reactors**
  - Eulerian multiphase (EMP)
  - Distinct element method (DEM)
  - Reactions
  - Accuracy versus time

- **Stirred reactors**
  - Robust meshing
  - Polymerization
  - Micro-mixing G-L, S-L

- **Bubble columns**
  - Size distribution
  - Large scale interfaces

- **Membrane separation**
  - Fugacity-based source/sink

- **High T process**
  - Process burners
  - Air ducts
  - Furnaces

Figure 11: Typical methods for reactor modeling in STAR-CCM+.
Conclusion

The capabilities available in STAR-CCM+ allow reaction engineers to look at the transport processes in various reactor types, including packed-bed reactors, fluidization, stirred reactors, bubble columns and membrane reactors, as well as all the various high-temperature processes in gas-phase reactions. Even in established processes, the underlying transport processes are crucial for reactor design and open up possibilities for improvement. For each of those transport processes, using STAR-CCM+ provides numerous ways and capabilities for modeling and discovering better reactor designs, faster.