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Computational Fluid Dynamics For The Chemical Process Industries

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Abstract:

The chemical process industries face new challenges as they enter the 21st century. To meet these challenges the chemical process industries are expected to integrate key technologies into their design and development processes. Computational Fluid Dynamics (CFD) has been identified as one of the key technologies for chemical process industries. This article provides an overview of computational fluid dynamics methods for the chemical process industries.

The chemical process industries involve a wide variety of process equipment and a process unit is required to perform a wide variety of duties. Hence, it becomes essential to predict its performance under a wide variety of operating conditions. The flow field involved is very complex and conventional methods of analysis are not adequate. Computational fluid dynamics provides a viable tool for analysis and trouble shooting of such equipment. A typical unit operation processes a large amount of fluid. Given the economics of most unit operations, even small improvements in efficiency and performance can result in a significant increase in revenue and savings in costs.

Introduction:

As the chemical process industries enter the 21st century they faces new challenges. The predominant forces of change include increased globalization of markets, demands for cleaner environment, higher customer expectations and increased profitability. There has been a general thrust to reduce waste and improve efficiency of processes in general. The traditional approach of taking a product from laboratory scale to pilot plants and then to production is no longer attractive. Process and product development are often initiated simultaneously, as a result, rapid prototyping and analysis is required. To meet these challenges innovation is required at all phases of product development. To meet these goals, Technology Vision 2020[1], a document highlighting plans for the chemical process industries for the next 20 years has identified three enabling technologies. Computational fluid dynamics (CFD) is one such technology that is expected to lead chemical process companies into the future. The integration of CFD methods will lead

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to shortened product-process development cycles, optimization of existing processes, reduced energy requirements and efficient design of new products and processes. Unit operations in the chemical process industries handle large amounts of fluid; as a result, small increments in efficiency lead to large increments in product cost savings. It is thus essential for not only the research and development staff in the chemical process industries but also for chemical plant managers and production managers to understand the benefits of CFD so that it can be integrated into the development process.

Companies are in the process of diversifying their products; as a result, the same process equipment is called on to perform various tasks. Table 1 summarizes the wide variety of process equipment in the chemical process industries [2] that can benefit from CFD analysis.

Fluid Moving Devices	Pipes, valves, pumps, compressors
Heat Generation and Heat Transfer Units	Boilers, furnaces, burners, process heaters, heat exchangers, condensers, evaporators
Drying Units	Spray dryers, pneumatic dryers, fluidized bed dryers, rotary drum dryers
Mixing and Agitation Units	Static mixers, stirred tank vessels
Mills and Classifiers	Rotary drum mills, gas-solid classifiers
Reactors	Tubular reactors, packed bed reactors, bubble column reactors, fluidized bed reactors
Separation Equipment	Cyclones, electro-static precipitators, hydro-cyclones, centrifuges, gravity separators

Table 1: Chemical process equipment that can benefit from CFD analysis.

To meet the challenges associated with the operation of a wide variety of process equipment, suitable analysis tools are required. The flow fields involved in chemical process equipment are very complex and conventional methods of analysis are not adequate. Experimental measurement is not always possible. While measurement probes provide point data, very often full-field data or data at multiple locations is required to fully diagnose a problem. Trouble shooting as well as improvements in efficiency and performance are typically achieved by trial and error based on past experience. Failure of chemical process equipment can result in undesirable downtime and loss of revenue. Hence, more adequate techniques of troubleshooting are required so that downtime can be minimized. CFD is a viable tool for analysis of chemical process equipment.

CFD methods are widely applied within various industries to examine fluid flow and heat transfer behavior. In the Aerospace industry, CFD is routinely applied for aerodynamic calculations, such as computation of lift and drag of lifting surfaces. In the automotive and heavy equipment industries, CFD is applied for external drag calculations, climate control and under-hood cooling. The heating and ventilation industry, power generation industry and chemical process industries, including oil and gas companies, chemical companies, pulp and paper companies and pharmaceutical companies are now beginning to apply CFD methods to gain insight into their various processes. The Aerospace industry has been applying CFD methods for the longest period of time. CFD methods in this industry are routinely applied to improve lift and drag of aerodynamic surfaces. The overall behavior of flow is very well understood and small improvements (on the order of 1%) are sought to achieve incremental increases in performance. In general, CFD methods are applied to understand the overall flow behavior. A typical CFD study is aimed at comparing different designs. 'What-if' studies are performed to examine the influence of various parameters on flow behavior and hence performance. Relative comparison of various designs is carried out using CFD methods. A number of conceptual design changes can be examined rapidly in a "virtual laboratory," without actually building a physical model. CFD study of a full-scale model can be carried out, thus eliminating scale-up issues. Unlike experimental methods, CFD provides full-field data. Pressure, velocity, density, temperature and other quantities of interest are obtained at each and every point in the simulated flow domain. These benefits make CFD a viable tool for analysis, design and rapid proto-typing. CFD can be integrated in the product cycle at various stages as shown in Figure 1.

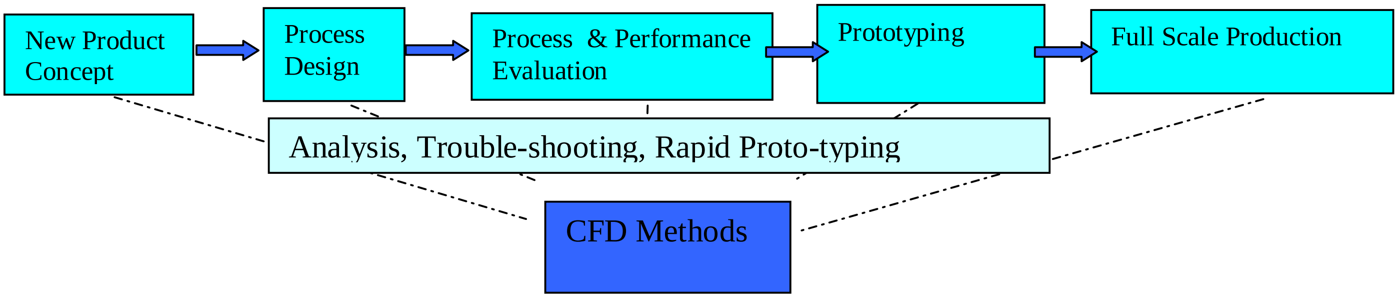


Figure 1: Role of CFD Methods

Overview of CFD Methods:

Computational fluid dynamics (CFD) methods are based on first principles of mass, momentum and energy conservation as described by the following equations:

Mass:

$$\frac{\partial \rho}{\partial t}+\frac{\partial u_j}{\partial x_j}= \text{Sm} \qquad (1)$$

Momentum: $$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} + \frac{\partial P}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j} + \mathrm{Sf}_i \qquad (2)$$

Energy: $$\frac{\partial \rho H}{\partial t} + \frac{\partial \rho u_j H}{\partial x_j} + \frac{\partial q_j}{\partial x_j} = \frac{\partial u_i \tau_{ij}}{\partial t} + \frac{\partial p}{\partial t} + \mathrm{Sh} \qquad (3)$$

Where ρ is fluid density, t is time, x is coordinate, u is velocity, P is fluid pressure, H is fluid enthalpy, τ is shear stress and $i, j, k = 1,2,3$ represent three coordinate directions. Sm is mass source due to reactions or other mass transfer mechanisms. Sf represents momentum source due to mass transfer, body forces such as gravitational force etc. Sh is energy source due to mass transfer, phase change and energy generation by other mechanisms.

CFD methods involve the solution of conservation equations for mass, momentum and energy at thousands of locations within the flow domain. These locations are created by generating a mesh. The equations are applied at mesh locations using discretization techniques. The details of these methods are described in references [4-5]. The computed solution provides flow variables such as velocity, pressure, temperature, density, concentration, etc. at thousands of locations within the domain.

A number of commercial CFD software packages are available. CFD solvers are wrapped in a user-friendly graphical interface (GUI). These general-purpose CFD software packages can be applied to simulate fluid flow, heat transfer, chemical species transport and reactions for a wide variety of applications. The look, feel, performance and accuracy may differ from one CFD package to another. However, the basic principles and steps involved in performing a CFD analysis is the same. CFD analysis can be broken down into three main steps, viz. Pre-processing, Solution and Post-processing. The main steps of performing a CFD analysis are depicted in Figure 2.

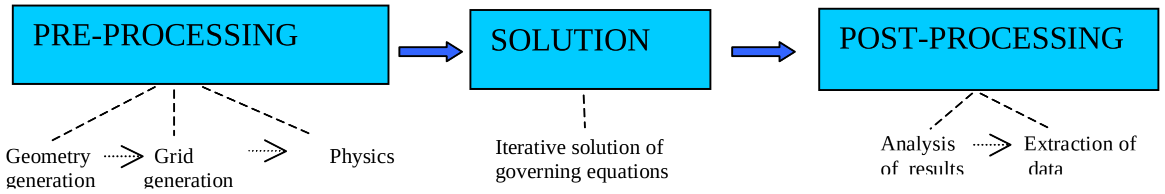


Figure 2: Steps of performing a CFD analysis

The first step in performing a CFD analysis is called Pre-processing. This involves identification of the flow region of interest, geometric representation of the region, meshing and definition of flow physics. Proper selection of the region of interest and appropriate simplifications play a key role in the success of the calculation. Once the region is defined, a computer model of the geometry is created. Most commercial CFD packages provide a CAD-like geometry generation engine. The next step is mesh definition. The governing equations are solved at discrete locations in the flow domain. These locations depend on the mesh resolution. The accuracy of a CFD calculation and computer time required for a solution are dependent on mesh resolution. User experience and skill play a crucial role in the choice of a suitable mesh. Appropriate boundary conditions are applied to define regions of inflow, outflow, walls and other important features. Physical models within the software are activated to simulate flow physics pertaining to the application at hand. For example, a turbulence model is activated to simulate turbulent flow. Selection of appropriate physical models and their applicability to the flow physics at hand is critical to the overall accuracy of a CFD solution.

Once the problem definition is completed it is submitted to the solver for computation of a solution. This step is the Solution step. The governing equations are coupled and non-linear in nature. Therefore guess-and-correct, iterative strategy is adopted to compute the solution. While the solution method is automated, user intervention is frequently required to obtain a stable converged solution.

The third step is Post-processing during which CFD results are analyzed. A CFD solution provides full-field data; flow variables at thousands, perhaps hundreds of thousands of locations are available. A representation of the flow field is created by plotting flow variables in space on a plane or a line or in a three-dimensional region of interest. The spatial plots give the analyst a ‘look inside’ the unit which is unavailable experimentally. However, the real value of CFD simulation is frequently found in its ability to provide accurate predictions of integrated quantities such as heat transfer rates, mass transfer rates and forces imposed on vessel internals. References [4-5] provide numerical details of mesh generation, discretization and CFD solver techniques.

CFD Applications in the Chemical Process Industries:

CFD applications to a number of unit operations and processes in the chemical process industries are described in the following sections.

CFD for Mixing Applications: Mixing processes form the heart of the chemical process industries. Mixing may involve blending of two streams of the same fluid but at different temperatures (thermal mixing) or, it may involve mixing of two or more different fluids with or without chemical reactions. The degree of mixing required and the equipment applied depends on the actual application. Static mixers for fluid-fluid mixing and stirred tanks are by far the most commonly applied units for mixing.

CFD methods are applied to examine the performance of static mixers. CFD solutions are applied to predict the degree of mixing achieved, thus indicating if more mixing elements are required. Figure 3a depicts surface mesh and blade orientation for a Kinecs mixer. Figure 3b depicts the mass fraction concentration of the two species being mixed. The degree of mixing is shown as the color proceeds from distinct inlet streams (red and blue) to the fully mixed outlet stream (green). The pressure drop, hence power required can also be derived from a CFD solution.

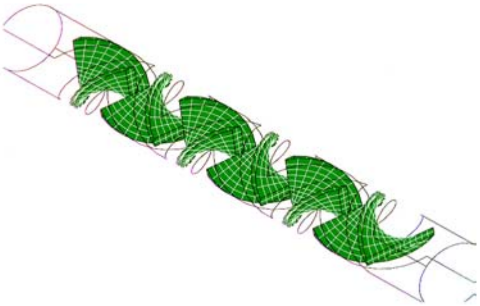


Figure 3a: Kinecs mixer, blade orientation

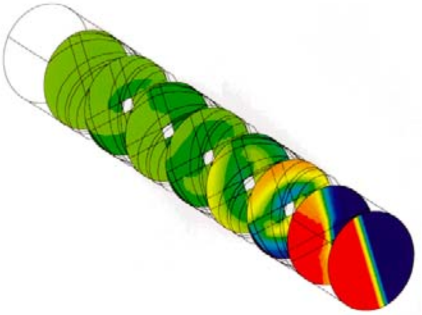


Figure 3b: Mass fraction contours

Stirred tank reactors are very commonly used in the chemical process industries for a wide range of duties. The primary function of these vessels is to provide adequate stirring and mixing of a mixture. The mixing characteristics influence the product quality and efficiency of the process to a great degree.

Stirred vessels come in various shapes, sizes and are equipped with many different types of impellers. Very often the same vessel is required to perform various duties and it is essential for engineers to ensure that adequate shaft power is available to perform the mixing duty. More importantly, it is essential to ensure efficient operation of the vessel for a given duty. This is very often accomplished by placing the impellers in the vessel at various locations. Empirical correlations for estimating vessel performance exist. However, these correlations are unable to predict the performance accurately and are very often based on the assumption of linear superposition of data.

The following study examines the influence of impeller location on the flow field. CFD methods are employed to analyze the flow field and study vessel flow characteristics. Single-phase flow in a flat-bottom, baffled tank with dual 4-bladed Rushton impellers is modeled. Rushton impellers are typically employed to generate radial flow. Figure 4a shows properly placed impellers in the vessel. The radial flow field generated by the impellers leads to formation of four torroidal re-circulation regions. The impellers in this case operate with little if any interaction between them. If the impellers are placed closer to each other, a converging flow pattern is generated. This is depicted in Figure 4b. The upper impeller pumps downward and the lower impeller pumps upwards. However, if the impellers are placed further apart, a diverging flow pattern as depicted in Figure 4c is generated. In this case, the lower impeller pumps downward and the upper impeller continues to pump radially outwards. Changes in impeller position lead to a drastic change in the flow pattern. This has a strong effect on vessel performance, mixing characteristics and hence product quality and efficiency. Impeller-impeller interaction is a strong non-linear effect and cannot be predicted by simple empirical correlations. CFD provides a viable method to analyze and optimize stirred tank performance. Impeller performance and flow field characteristics can be successfully predicted using CFD methods.

CFD methods can also be applied to predict shear stress distribution within a stirred vessel. This is important for dissolution, emulsification and dispersion. Shear stress distribution is also important for biomedical applications where excessive shear may lead to damage of product and loss of efficacy.

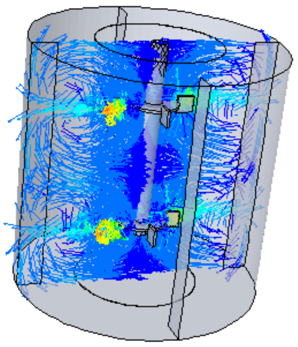


Figure 4a: Stirred tank, radially pumping impellers

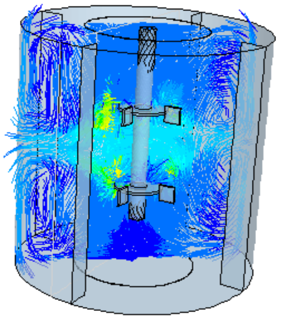


Figure 4b: Stirred tank, closely placed impellers

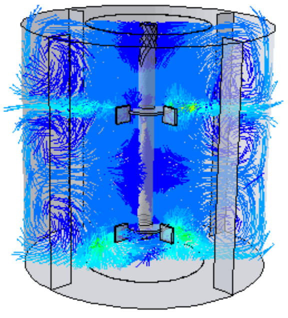


Figure 4c: Stirred tank, impellers too far apart

CFD for Fluid Transport Devices: CFD methods have been applied for analysis and performance prediction of fluid transport devices such as pumps, compressors and fans. Pumps are commonly employed in the process industries for transport of fluids. Increasing demands for greater productivity very often calls for the same pump to handle different fluids. In the following study CFD techniques are employed to predict pump performance under different operating conditions. Typical flow field is depicted in Figures 5a and 5b. The accuracy of CFD solution is demonstrated through detailed comparison with experimental data as shown in Figure 6.

Figure 5a: Pump, velocity distribution

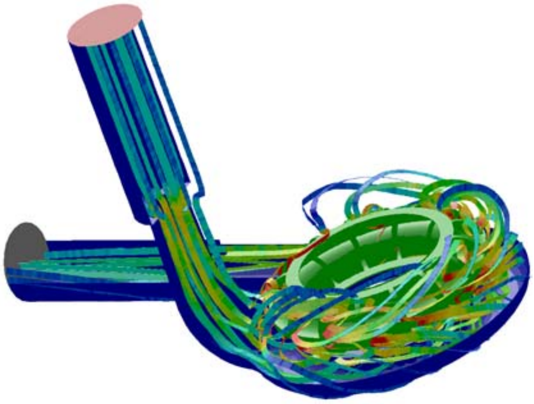


Figure 5b: Pump, streak lines

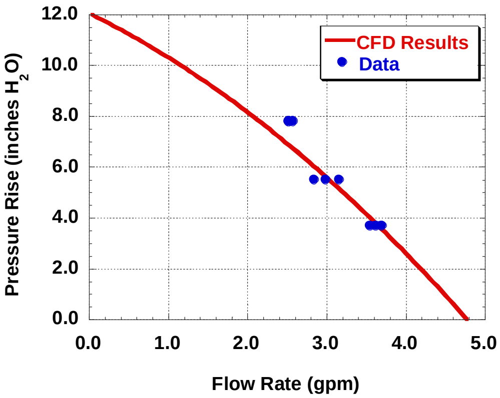
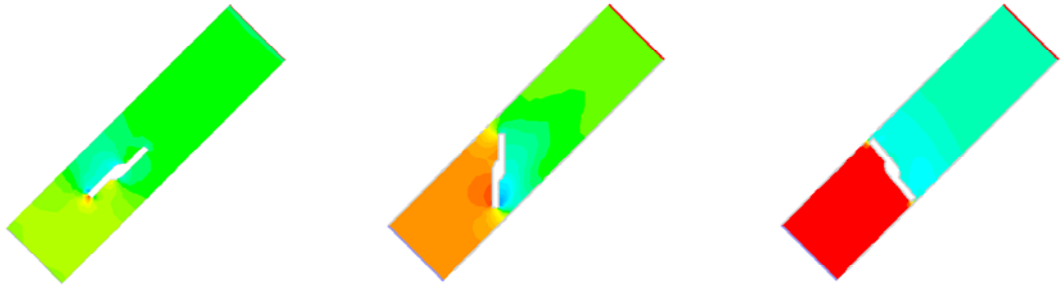


Figure 6: Pump performance curve, comparison of CFD results with experimental data

CFD methods are also employed to derive input information for other solution tools. Figure 7 shows how CFD techniques are employed to obtain pressure distribution and flow characteristics of a butterfly valve. The discharge coefficient vs. angle computed using the CFD model is applied as input to a waterhammer calculation tool. The resulting waterhammer pressure profile is depicted in Figure 8.



Pressure @ 0 Degrees **Pressure @ 45 Degrees** **Pressure @ 85 Degrees**

Figure 7: Butterfly valve, pressure distribution for various positions

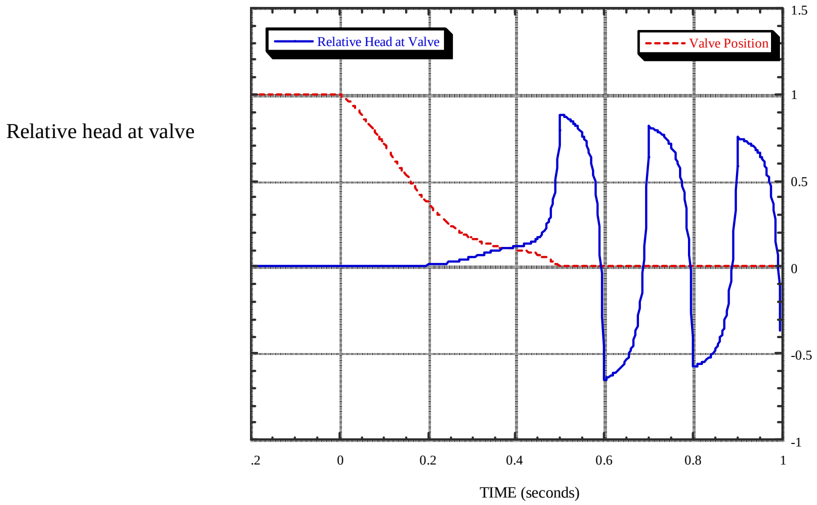


Figure 8: Butterfly valve, Waterhammer profile

Pneumatic transport of products in the form of powders is very common in the chemical process industries. Granular solids of free-flowing natures may be conveyed through ducts with high velocity streams. Air-conveyed materials include chemicals, plastics, pellets, grains and powders of all kinds. Transfer of catalysts between regenerator and reactor under fluidized conditions is a common pneumatic solids transport process. The performance of pneumatic conveyors is sensitive to several characteristics of the solids such as bulk density and particle size distribution. Pressure drop, power requirements are key indicators of performance. Erosion caused by particle impact is an area of concern. Figures 9a and 9b depict particle paths for heavy and light particles in a pneumatic conveyer junction. Heavy particles impact the walls of the junction thereby increasing the risk of erosion.

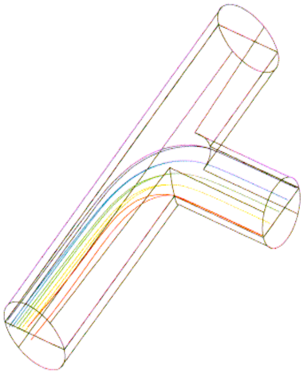


Figure 9a: Pneumatic conveying, light particle tracks

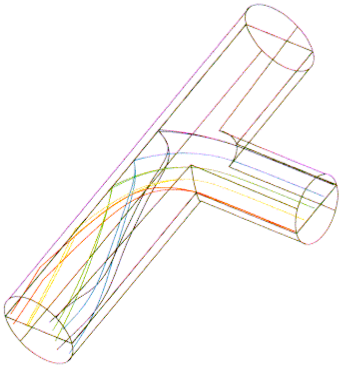


Figure 9b: Pneumatic conveying, heavy particle tracks

CFD for Separation Devices: CFD techniques are employed for analysis of separation devices such as cyclones, electro-static precipitators, and scrubbers. In the following study CFD methods are employed to optimize and predict performance of an existing cyclone design. CFD solutions depict particle paths for various particle sizes as shown in Figure 10a and 10b. CFD techniques were employed to perform 'what-if' analysis for optimization of the design. The performance computed using CFD methods closely matched that observed in physical testing wherein 90% of 10 micron particles were removed while only 10% of 1 micron particles were separated from the air stream.

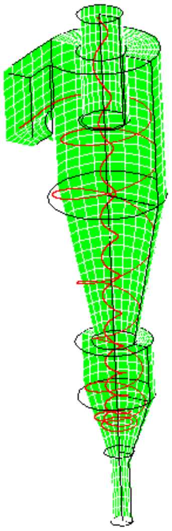


Figure10a: Cyclone, path line of 1μ particle

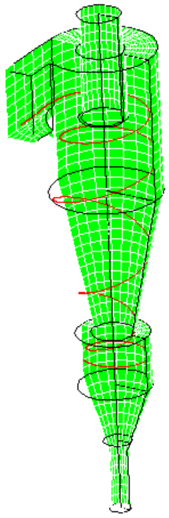


Figure10b: Cyclone, path line of 10μ particle

Electro-static precipitators (ESP) are very effective in the removal of fine mists and fine particles from gas streams. Atmospheric dust concentration measurement is also achieved by employing electro-static precipitators. A typical electrostatic precipitator is comprised of ductwork and a diffuser section. Electro-statically charged filters are located in the diffuser section, effective performance of an ESP requires uniform flow in the diffuser section. The upstream ductwork can have a significant impact on the flow entering the diffuser and hence its effectiveness and performance. These devices are several meters in dimensions and are difficult to prototype. Expensive experimental setups may be constructed to study flow field in such devices. The other option is numerical simulation of flow field. This option is relatively inexpensive and can be completed on a shorter time scale. CFD methods are routinely employed to examine ESP performance.

In the following study, CFD is applied to examine the effect of various distributor plate configurations on the uniformity of flow entering the diffuser section of an ESP. The original design employs a grid-type distributor plate as shown in Figure 11a. As depicted in Figure 11b, the flow entering the diffuser is not uniformly distributed and continues as a jet in the core of the diffuser section. This leads to a large recirculation region in the ESP. The effect of a grid employing three vertical and three horizontally placed splitter plates is examined. This configuration is shown in Figure 12a. The velocity field in the ESP, as depicted in Figure 12b is more uniform but the recirculation region is not entirely eliminated. CFD methods can be rapidly applied to examine the effect of various geometric and flow parameters on the overall flow behavior in an ESP. These techniques can be applied for trouble-shooting, improving the performance and also for rapid prototyping.

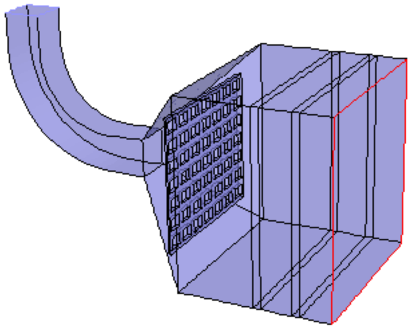


Figure 11a: Electro-static precipitator

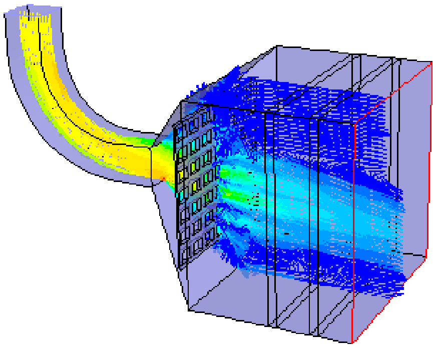


Figure 11b: Electro-static precipitator, velocity field

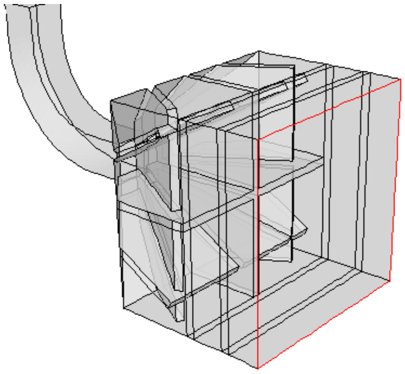


Figure 12a: Electro-static precipitator, modified configuration

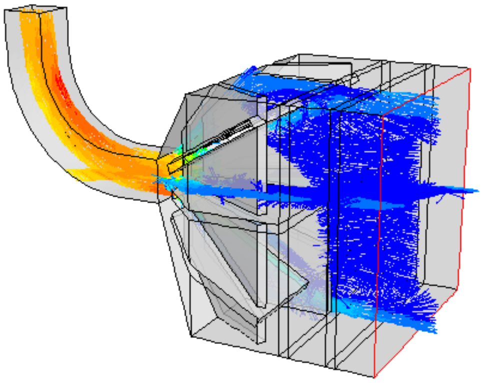


Figure 12b: Electro-static precipitator, modified configuration velocity field.

CFD for Dryers: Drying equipment is usually large and expensive. As a result, efficiency is an important factor that influences production and operation cost. In this section the benefits derived from CFD study of a spray dryer are discussed.

CFD is used to analyze the performance of an industrial spray dryer in advance of making major structural changes to the dryer. The risk of lost profit during changeover (especially if the improvement did not materialize) is minimized. CFD is applied to examine configuration changes and thus minimize risk and avoid unnecessary downtime during testing. The velocity distribution depicted in Figure 13 shows skewed flow. This is a result of uneven pressure distribution in the air dispersing head. CFD models are applied to determine optimum equipment configuration and process settings. CFD results can provide the necessary confidence that the proposed modifications will work before capital equipment is ordered and field-testing scheduled.

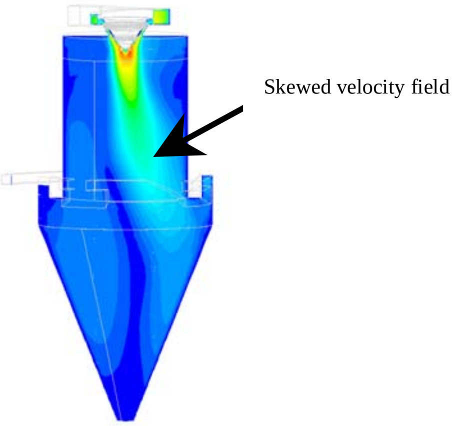


Figure 13: Spray dryer, velocity field

CFD for Heat generation and Heat Transfer Equipment: Heat transfer equipment such as heat exchangers are employed throughout a chemical processing plant. Failure of this equipment can lead to downtime and significant loss of revenue. Hence, it is essential for this equipment to perform as reliably as possible. Inefficiencies associated with heat transfer equipment directly influence production cost. Small increments in improved efficiency can result in significant reduction of operating cost and increased revenues. CFD techniques can provide an insight into the function of these devices and can help identify areas for improvement. Figure 14a shows the temperature distribution over an array of cylinder in cross flow. This is a very common configuration in heat exchangers. Comparison of CFD results with experimental data is depicted in Figure 14b.

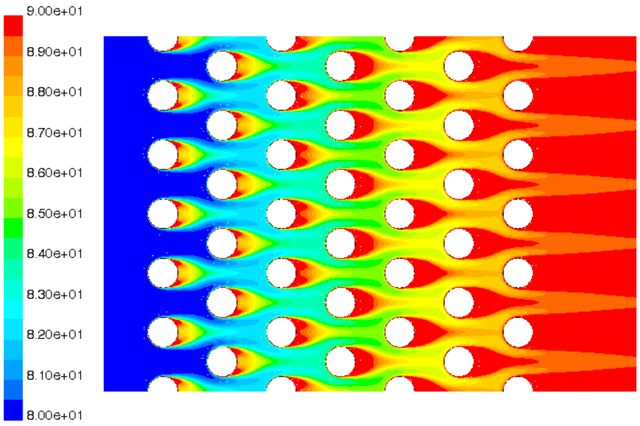


Figure 14a: Heat exchanger, temperature distribution

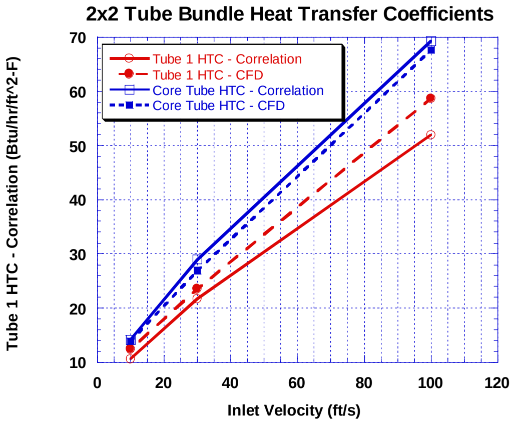


Figure 14b: Comparison of CFD results with data

Process heaters of various types are employed for endothermic reactions. The two major types of heaters are direct-fired or indirect-fired. Direct-fired heaters are typically employed for hydrocarbon reforming, pyrolysis-type of processes. High process temperatures are achieved by direct transfer of heat from the products of combustion of fuels. Heat is released by the process of combustion which is transferred to fluids inside tubes which are arranged along the walls and roof of the combustion chamber.

Tubes containing the process fluid are subject to combustion process gases and high temperatures. If the heating is not uniform then hot-spots may occur leading to failure; on the other hand, inadequate heating can lead to lower process fluid temperatures and inefficiencies. Formation of pollutants such as NOx can be reduced using design guidance provided by CFD simulations.

The combustion process and heat transfer within direct-fired heaters are very complex. Simple methods are inadequate to analyze and predict performance. Experimental measurements are difficult and even impossible. Computational methods such as CFD present a viable approach for analysis of such equipment.

The combustion process and heat transfer in a direct-fired heater are modeled using computational fluid dynamics. A vertical-cylindrical radiant process heater is modeled. The tubes containing the process fluid are arranged helically as a coil along the walls of the combustion chamber. Firing of fuel is vertical from the floor. Heat transfer to the process tube and uniformity of the temperature field are examined and depicted in Figure 15, red regions denote high temperature and blue regions correspond to low temperature. It is observed that the heat transfer to the tubes is quite uniform. However, the exhaust gas temperature is high, indicating that a heat recovery unit downstream of the primary heater may need to be installed to recover waste heat.

Figure 15: Process heater, temperature distribution

Flame stability and burner efficiency are very critical to the proper functioning of a process heater, power plant or furnace. Flame length, shape and size can influence the process. If the flame is too long it can impinge on critical regions of the apparatus and cause thermal damage, if it is too short it may wear out the burner tip. Replacement of the burner or associated apparatus results in downtime and loss of product revenue. Computational fluid dynamics modeling methods can be applied to gain insight into flame characteristics. Appropriate burner configurations can be arrived at through computer modeling. In the present study a natural gas burner is modified. The flame length, shape and size are examined for two burner configurations. In this case fuel injection lance modifications are examined to study the effect on flame length, shape and size. The fuel lance tip is modified. Introduction of a disk at the lance tip to inject fuel gas through a conical slot results in a much shorter flame and desirable characteristics.

This effect is depicted in Figures 16a and 16b. Red regions denote high temperature and blue regions correspond to low temperature.

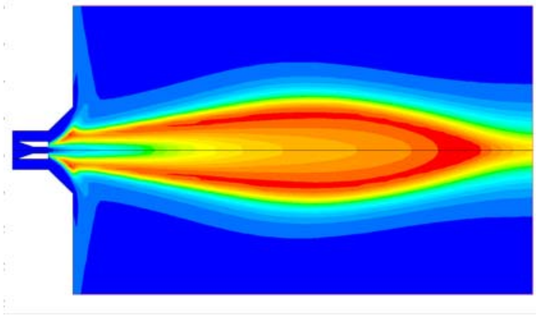


Figure 16a: Burner, flame profile

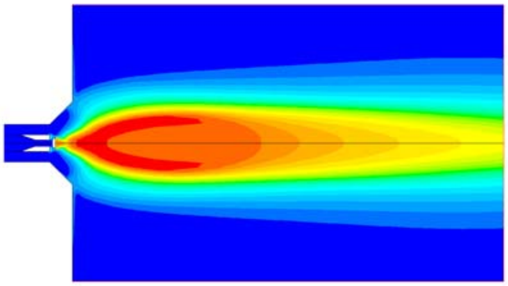


Figure 16b: Burner, flame profile
fuel lance tip modified

CFD for complex multi-phase flows: CFD techniques are also applied to examine flow behavior in more complex systems such as bubble column reactors. These are gas-liquid systems and CFD simulation techniques for these applications are more involved and sophisticated. CFD methods have evolved over the past few years enabling simulation of multi-fluid systems such as fluidized bed reactors (FCCU) and risers. CFD methods have helped eliminate sloshing and spilling during filling processes. Figure 17 depicts filling of a container. This plot is typical of solution results that are used to optimize filling processes to increase throughput and reduce foaming.

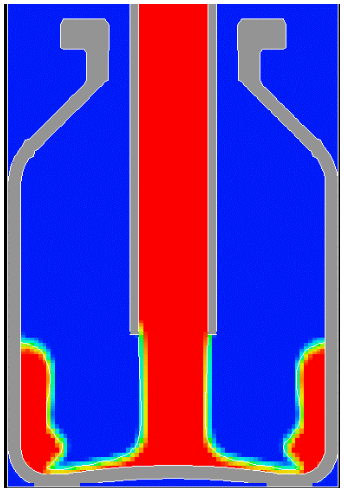


Figure 17: Container filling process

Conclusions:

Technology Vision 2020[1] has identified CFD as a key technology that will enable the chemical process industries meet challenges of the future. The integration of CFD methods will lead to shortened product-process development cycles, optimization of existing processes, reduced energy requirements and efficient design of new products and processes. Unit operations in chemical process industries handle large amounts of fluid, as a result, small increments in efficiency lead to large increments in product cost savings, CFD solutions can help accomplish this. The number of processes that can be improved with the aid of CFD techniques are many. Aerospace and automobile industries have already integrated CFD methods into their design process. Chemical process industries are now beginning to accept this technology; however, it is yet to be fully integrated. The potential for process improvements using CFD solutions is yet to be realized.

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