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Multidisciplinary simulation and design exploration in the chemical and process industry

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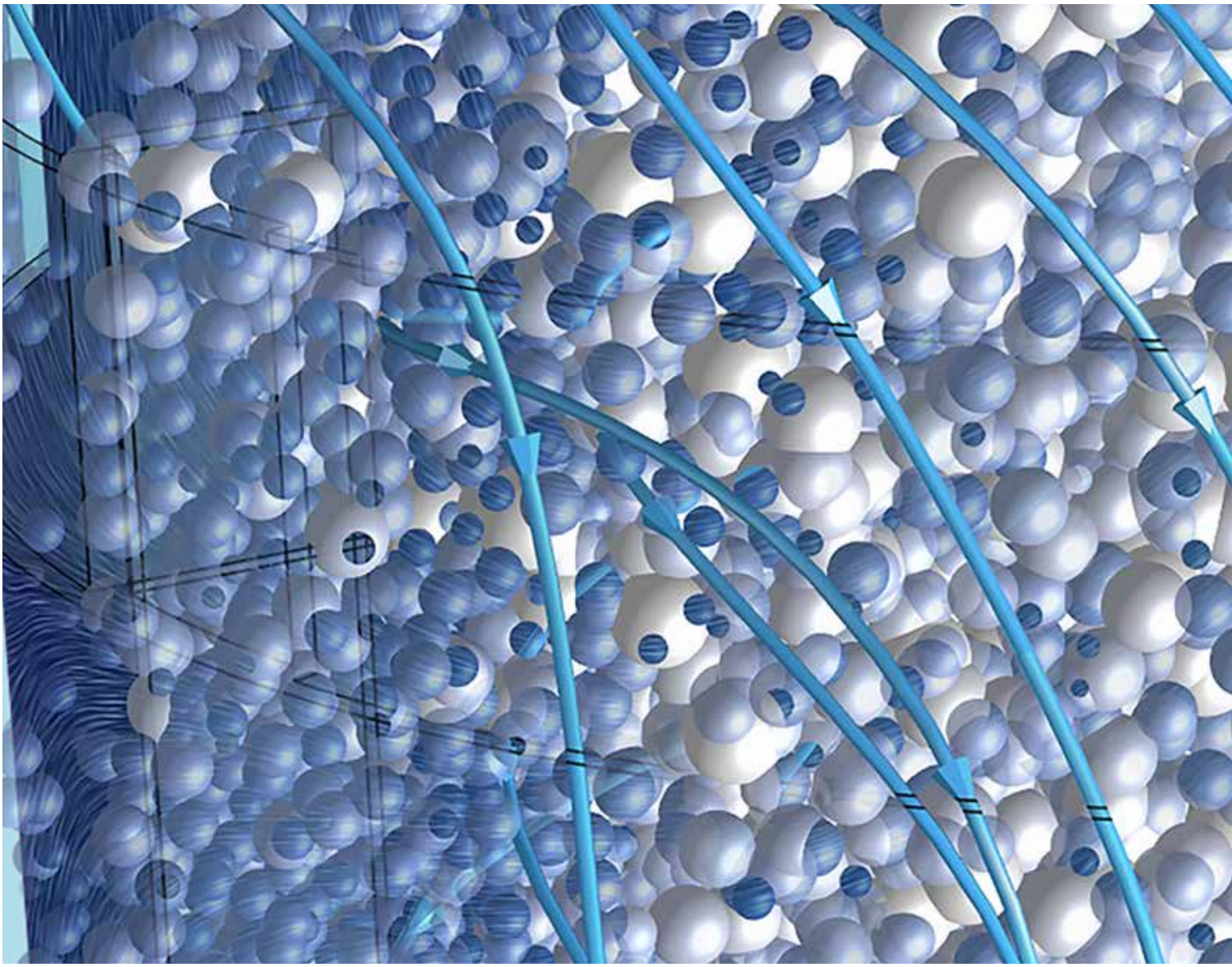

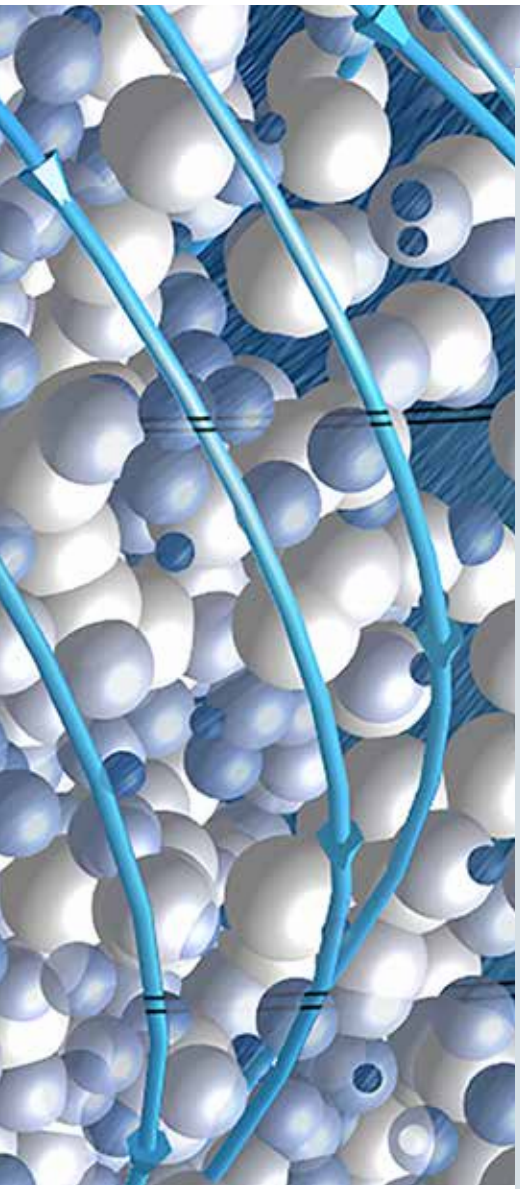

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Introduction

Ravindra Aglave
Director,Chemical and Process

The chemical and process industry manufactures functional products from raw materials. These materials form the basis of new functionalities in a host of other industries: from touch sensitive glass for smartphones, corrosion inhibitors for oil pipelines, paints and foams for automobiles to carbon fibers for aircraft.

Historically, civilizations have progressed due to their ability to find, process and apply materials for tools and utensils for household use in everyday life and as means of transport. Chemical and process engineering expertise started in the Stone Age and continued through the Copper Age, Iron Age, etc., and onto the present day. In fact, it was described with one word, "plastics," in the film, *The Graduate*.

Taking a raw material of relatively low value, converting it into a material of high value through reactions and eventually separating out the wastes and unwanted products is the basis of any process in the chemical industry. In the past, the design and details of these processes were mostly done via experience. Chemical engineering emerged as a science and a branch of engineering in the early 20th century when the need for materials such as rubber, fuels and explosives was high during World War I and World War II. Fundamental equations to describe the chemical industry processes were developed, complemented by experiments and used to derive correlations for phenomena that were difficult to describe mathematically. At this time the three major tools at the disposal of chemical process engineers were experiments, analytical calculations and experience.

The first process simulation tools were created in the 1970s with the advent of computers. In the 1980s, new numerical analysis methods were developed, led by the aerospace and automobile industries. Computational fluid dynamics (CFD) allowed engineers to test their "raw" designs and verify them without building physical prototypes. CFD use developed rapidly in the automobile and aerospace industries, as design in these disciplines was highly influenced by fluid flow and heat transfer. In comparison, in the chemical industry, innovation is driven by chemistry at the molecular level.

At this time the micro-scale processes involved in chemical processes were not well enough understood to create CFD models. In recent years, however, significant research has advanced the micro-scale models and enabled a deeper and wider application, especially in combustion reactions (applied both to internal combustion engines or otherwise). Developments for many other processes such as crystallization or lyophilization, are also ongoing in academic circles. This rapid pace of research has been reflected in our rapid development of

Simcenter STAR-CCM+™ software. Just in the span of a few years, many of these new capabilities have been implemented and validated (or are on the verge of implementation), causing a big leap in the capability of the software. Simcenter STAR-CCM+ now essentially bridges the gap between the large scale transport processes (mass, heat and momentum transfer) and the micro-scale chemical processes, allowing engineers to investigate the effects of the large scale processes on product quality and yield.

Simcenter STAR-CCM+ makes simulation accessible to process engineers with limited simulation experience but strong process knowledge. Combined with Simcenter STAR-CCM+ Mixing Vessel Workflow, a dedicated tool for mixing, Simcenter STAR-CCM+ offers a virtual process design and development platform. With this step-change in capabilities, I wouldn't be surprised if CFD simulation becomes as commonplace as process simulation is today in the chemical industry. And there is no doubt about the value it will bring to the business:

- Freedom to test novel concepts to meet process needs
- Ideas and solutions can be tested under actual operating conditions and scales
- Scale-up of processes from preliminary design and pilot scale knowledge

The insight gained from simulation is now accessible to a much wider set of engineers. Just as many process engineers graduate today from college with experience in process simulation tools, we expect that future graduates will be arriving in the industry with a good understanding of deploying not just process simulation but also CFD and discreet element method (DEM) simulation. This flood of knowledge and skills will make the industry more cost efficient, less polluting and ultimately more innovative.

"Simcenter STAR-CCM+ makes simulation accessible to process engineers with limited simulation experience but strong process knowledge."

Simcenter STAR-CCM+ Mixing Vessel Workflow: Because sometimes you want things “stirred, not shaken”

Ravindra Aglave
Director,Chemical and Process

Fascination with the martini

My first encounter with mixing was when I watched my first Bond movie as a boy. “Shaken, not stirred!” exclaims James when he orders a martini. I couldn’t understand why he would not want it stirred or completely mixed. It was only a case of a single impeller in a conical bottom vessel, with a liquid fill level a third of the height of the vessel. To simplify, a passive scalar could have been used to represent the second liquid. Q was completely capable of making a device that could fit in Bond’s iPhone or gear. My engineering genes were trying to peep out at a young age. Mixed drinks were not the norm in the country I grew up in, so the effect of delayed mixing on the taste and the subsequent evaporation on the palate were all unknown to me. But every time I watched a Bond movie, I used to wait for that moment.

Solving engineering problems

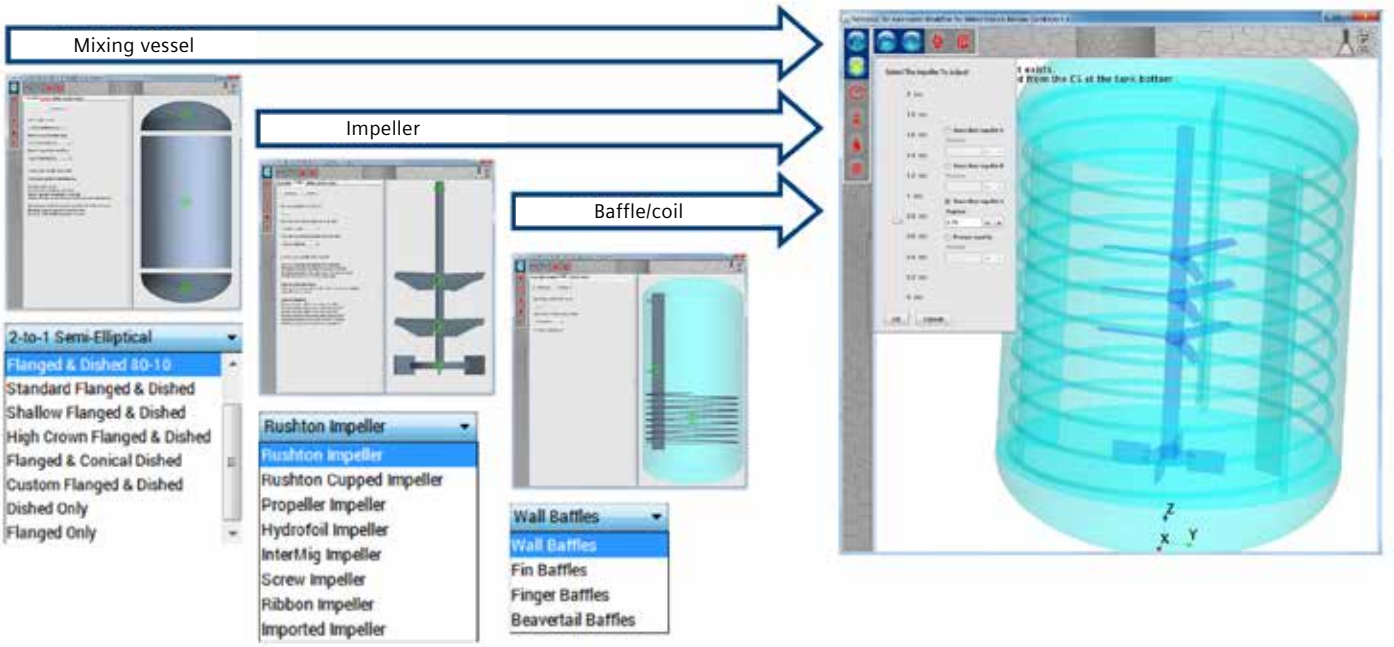
My fascination with how things work, especially chemical interactions, led me to eventually become a chemical engineer, specifically in the reaction/combustion field. The issue of mixing now popped up with more serious and professional needs. Learning modeling and CFD simulation gave me ways to look at those phenomena more fundamentally. When it came to mixing in stirred vessels, there was still a vast gap between going from the basic information of geometry and material data to the point where one could start a simulation. How would a genius like Q, who uses a mix of virtual and physical prototyping, address this problem? Would he encounter hurdles? Perhaps he would face the following issues:

- Creating even slightly complex geometry is time-consuming
- Steep learning curve because a set of good practices is missing
- Mature users don’t leave knowledge behind when they move to other fields
- Post simulation analysis is time-consuming

More than a point simulation

This is essentially what prompted me and my colleagues to conceive, design and create a virtual product development (VPD) tool for performing mixing simulations: Simcenter STAR-CCM+ Mixing Vessel Workflow. It walks a user through the essential steps in a seamless way.

Each step gives the user an option of entering the information at hand such as geometry parameters, choice of mesh types, material properties, etc. There is a host of standard impeller types that can be created in a flash or a computer-aided design (CAD) geometry can be imported. There are possibilities to set up multiphase (G-L, S-L, miscible L-L) simulations



as well, with best practice values automatically selected. A single point or multi-point sparger can be set up if desired. The user, however, has the choice of making any tweaks or tuning of the setting from the created SIM file directly in Simcenter STAR-CCM+.

Better design, faster!

The key value, however, comes from two things:

1. Postprocessing of results that are automated for typical plots, contours, etc. This is combined with the ability to include tracer analysis. All of those results are exported to Excel for further ease of analysis.
2. The created geometries are automatically parameterized. This means a user can run a design space exploration study with as much effort as a few drop-down menus and clicks.

If there ever was a time for chemical or process engineers (with no previous simulation or CFD background) involved in mixing process design, development and scale-up, then it would be now! Simcenter STAR-CCM+ Mixing Vessel Workflow will drop the barrier for engineers, no matter if they are in operations, engineering, development or research, and are active in the field looking to solve problems and optimize processes. They can introduce simulation with the help of Simcenter STAR-CCM+ Mixing Vessel Workflow as a modern engineering tool in their toolset of problem solving and keep on expanding its applicability based on the strength of a wide variety of multi-physics capabilities in Simcenter STAR-CCM+. If James Bond were an engineer rather than a slick spy, he would certainly be saying, “Stirred, not shaken!”

CPI Looks to the future

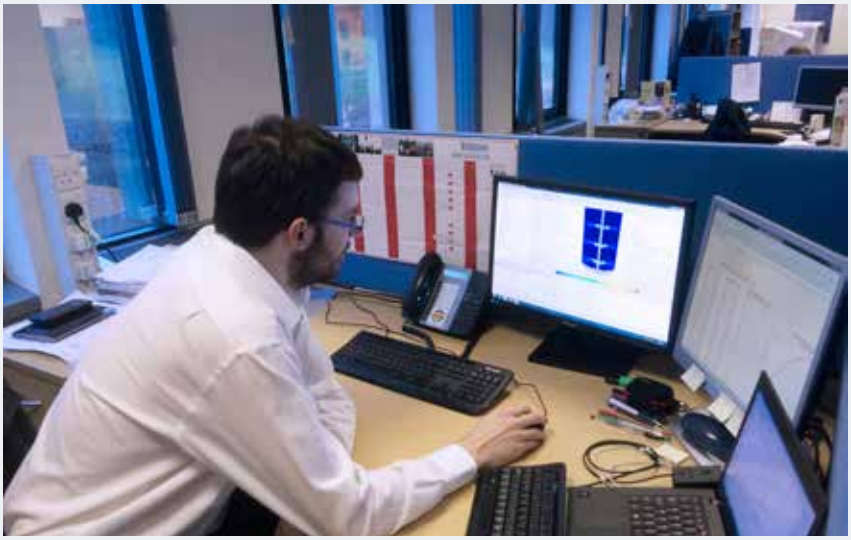


Figure 1: Alex Smith, senior process engineer at CPI.

Recently, I sat down with Alex Smith from the Centre for Process Innovation (CPI), a United Kingdom-based technology innovation center that uses knowledge in science and engineering combined with state-of-the-art facilities to enable their clients to prototype and scale up the next generation of products and processes. Smith is a recent recruit who is just approaching his first work anniversary with CPI. He is a senior process engineer within their Industrial Biotechnology and Bio-refining (IBandB) unit and it hasn't taken him very long to get his hands dirty with simulation work. He is currently balancing his time mostly between developing their CFD capability, both in model development and training of future users, and working on some more "standard" process engineering tasks, such as plant improvement and troubleshooting exercises.

This sounds like a very sensible and sustainable approach to developing a simulation capability, particularly in a company that is investing in CFD simulation for the first time. I asked Smith why CPI had decided to invest in a CFD simulation capability. "As a company in our position, assisting with the development of exciting and often unusual new processes it," he said, "it is important that we have access to cutting-edge tools and techniques to help us get the best results for our customers. With that in mind, the company placed a focus on improving our modeling and simulations capability in general, and the introduction of CFD modeling is just one part of this ongoing capability development."

Philosophy of simulation

When asked about CPI's philosophy of simulation, Smith went to pains to point out that CFD is a tool that builds upon traditional expertise, and that it supports but does not replace it: "When selecting conditions for trial runs, we primarily rely on the experience and judgment of the technical and operations teams. A validated model for a piece of equipment allows us an additional insight into the likely outcomes of a trial before it is run, and gives those experienced people extra tools and information to help them to select the most appropriate trials to run."

In a similar vein, CPI's CFD simulations are being used to improve physical testing, not replace it: "Computer-based simulations can't replace real-life testing," says Smith." The purpose of the model is to improve the focus of the live testing in order to make the process more efficient by giving an impression of how the equipment will perform before testing begins. This way the live testing can begin from a more appropriate starting point and less time will be spent running unnecessary or inappropriate trials on the equipment."

Future development

Although this CFD capability is still rather new to CPI, Smith and the team have a clear vision for the future development of their CFD capabilities across the business: "At CPI, the first application for CFD modeling is to generate validated models of our existing equipment for the purposes of improving our understanding of the equipment we currently operate, and therefore allowing us to simulate other scales outside of the available plant scales here on site. Initially, the focus is to

develop models that can accurately predict mixing behavior in our stirred tank reactors, and in the future we will also look into oxygen transfer and other key process attributes."

Eventually, CPI aims to expand the use of CFD modeling outside of IBandB to the other business units within the company. The business units of CPI all operate in different fields so it is important that the simulation software they use is adaptable and can cover a wide range of conditions and problems. Smith says,:"Within IBandB we aim in the long term to use CFD modeling as a design validation tool for new and novel reactor designs, whilst also using the package for troubleshooting and general plant performance improvements."

Alex pointed out that one of the most interesting features of working in a company like CPI is that you never really know what's coming next. He added: "The objective of the company is to help people and companies to develop their processes from laboratory to production scale, so the challenge really is to be able to constantly adapt to new processes and ideas which are coming out of universities and SMEs."

Why Simcenter STAR-CCM+?

Before choosing a CFD provider, Smith and the team at CPI went through a fairly extensive software selection process that finally resulted in them choosing Simcenter STAR-CCM+ software. Smith says,: "There are a few features in Simcenter STAR-CCM+ that we find particularly beneficial, for example, live monitoring of a solution as it develops can be a big time saver as it allows us to quickly see whether a model is on track or not without having to wait for the run to finish." Users at CPI also have been particularly impressed by the ease of use of the package in general: "The all-in-one window approach keeps things simple and tidy and is very intuitive to use," Smith says.

The fast pace of product development and the willingness to develop the program based on customer demand (IdeaStorm) is a particularly strong benefit for CPI. Smith comments, "We can see that the capabilities of the software are constantly improving and looking back over previous releases, more often than not each new release comes with new features that we find useful, rather than just superficial improvements." He also states that

Figure 2: Industrial biotechnology and bio-refining (IBandB) at CPI.

having a dedicated support engineer (DSE) is particularly beneficial to them: "We can be confident that when we do need to rely on technical support, our engineer will have a good understanding of our needs."

When I asked Smith to comment on what sets Simcenter STAR-CCM+ apart for CPI, he didn't hesitate to say: "For us it is not necessarily the physics models, it is more the ability to adjust those models on the fly, whilst monitoring the effect of those adjustments on the solution as you go. This way whilst a model is running, the physics conditions and model selection can be refined, and the effects of those refinements can be visualized instantly. Combined with the very strong postprocessing capability of Simcenter STAR-CCM+, this allows us to develop models that closely mimic reality relatively quickly, and without the need for a time-consuming iterative process to refine mesh and physics settings."

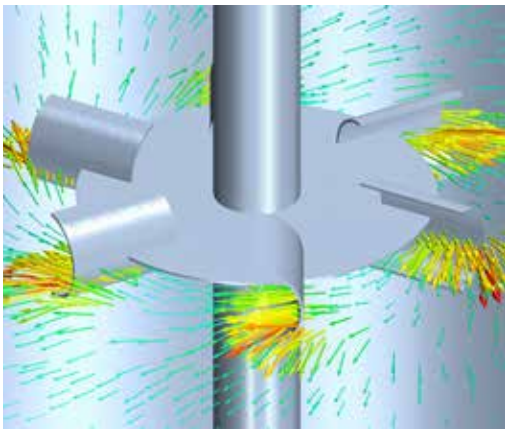


Figure 3: Predicted 3D flow pattern around impellers of a mixing tank using Simcenter STAR-CCM+.

From micro scales to macro scales/lab scale to plant scale

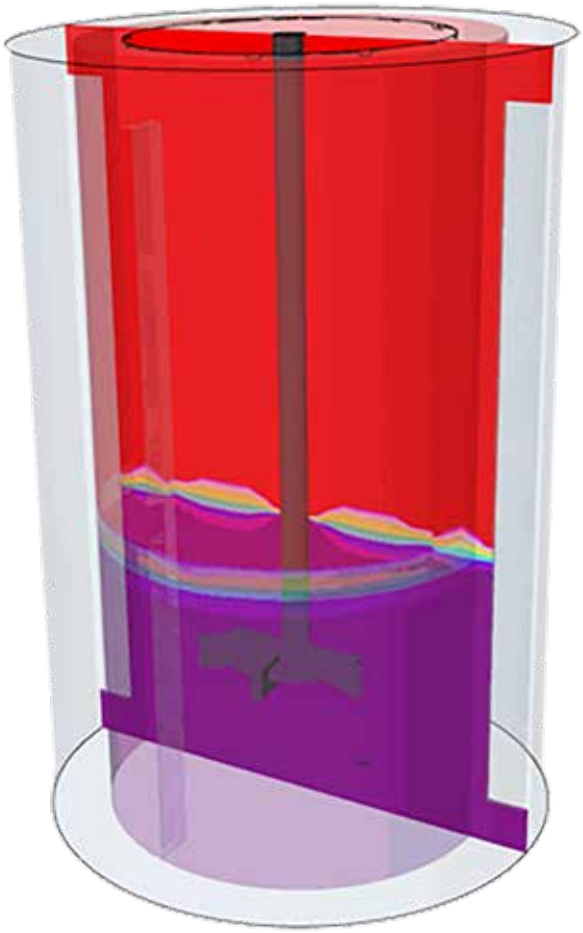
As anyone who has ever raised a child will know, parenting (in whatever form) is a scale-up problem. Each child is the product of many complex and interacting variables. Some of the obvious ones include: likes and dislikes, temperament, learning preferences and emotional, social and physical needs. None of these are constant, and all of them change as the child grows. Most people deal with this challenge with the help of more experienced parents and caregivers, by reading books on parenting, or most often of all, good old trial-and-error.

If we called a child a system (please don't tell my wife I just did that), what is fundamental is to understand the system behavior. Unfortunately, unlike an industrial scale-up problem, the system does not follow any rules of physics, instead following the much less predictable rules of psychology.

Either way, one can always imagine how the scaled-up system (how would you want your child to behave as an adult?) would behave based on expected outcomes from the process. This behavior is inherently tied to the physics governing the system. It is, however, quite common to perform trial-and-error procedure to understand the behavior rather than trying to a build relationships between the variables governing the system. Although it would be impossible to perform that for a human, it is difficult but doable for a given industrial system. It can be done in various flavors such a 1D model considering only part of the physics and assuming rest to behave ideally (for example, if a child learns to read and write, ideally he or she will be able to communicate).

Alternatively, it can be done at a more detailed 3D level (for example, a person needs to learn to read and write but also understand what is needed to interact with a variety of humans to communicate effectively).

The examples above can be equated to the design of an equipment which two streams are being added. It can be designed to carry out a reaction based on a model for reaction in 1D. The underlying assumption is the streams should mix themselves in an ideal manner. You will now realize that it is far from what is reality, just as it is to expect someone to communicate well if he has learned to read and write. Let us take the



simile to a further level of complexity. The skill of reading/writing is a micro scale phenomenon. The skill of communication is a macro scale phenomenon. The degree of communication at macro scale defines which variables/skills at micro scale are necessary. We can try to imagine a process of crystallization in an industrial crystallizer where the formation of crystals is dependent on concentrations, shear and other variables at micro scale. On a macro scale, the overall flow and heat transfer is affecting how the necessary variables are governed at micro scale. Almost all of the processes in chemical and allied industries consists of macro and micro level phenomena, and almost all of them need a scale up from a lab environment to a plant environment. Business dictates what the outcome from the plant should be. Research drives how the micro scales affect and govern a particular process. Simulation fills the gap of scaling up.

There are numerous examples and ways in which it has been utilized successfully, especially for difficult-to-understand processes and children. It perhaps has the role of a parent.

A virtual plant with Simcenter STAR-CCM+

Computational fluid dynamics (CFD) is a proven tool for the detailed design of equipment and plants. The main advantage of numerical simulation is that three-dimensional flow information can be generated to explore optimization possibilities. Tetra Pak CPS uses Simcenter STAR-CCM+ software to carry out this process.

A virtual plant

Specialized engineering and simulation software are important innovation tools. Today at Tetra Pak CPS, both basic engineering (collecting key data from a process) and detailed engineering (designing and optimizing the pipelines and individual components of a plant) are carried out via computer-aided engineering (CAE). The result is a digital representation of the plant, ideally as a 3D CAD model.

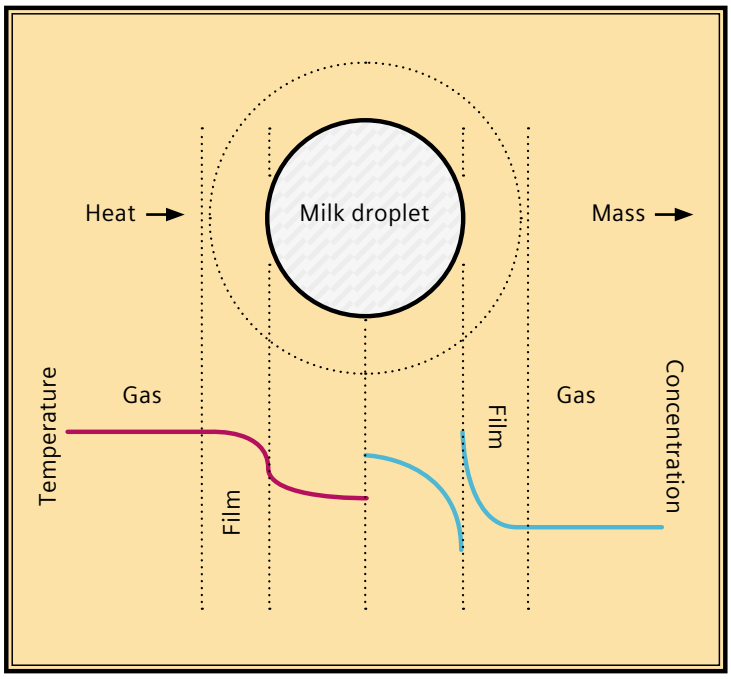
With CAE, it is now possible to virtually perform experiments that previously required elaborate laboratories or pilot plants, making it easier to compare alternatives, carry out marginal analyses and therefore support the optimization process. That means that the idea-to-product cycle is considerably sped up, which results in significant savings both in terms of time and elimination of costly physical experimentation.

CAE at work

The fact that CAE offers an efficient and cost-effective way to optimize equipment and plants proved decisive in convincing Tetra Pak to use this tool. This is because their customers, who are operators in the food industry, place a great deal of value on continual improvement: their goal is always to produce better products in increasingly smaller plants while reducing their production, operating and service costs.

One of the tools Tetra Pak CPS relies on is Simcenter STAR-CCM+ from Siemens Digital Industries Software. As Alfred Jongsma, manager of research and development (R&D)

The unique way in which Simcenter STAR-CCM+ is set up means the learning curve is really short.



Drying process in a spray dryer (heat and mass transfer).

at Tetra Pak CPS says: "We actively use Simcenter STAR-CCM+ for design optimization, troubleshooting and research and development projects."

The company has extensive experience using Simcenter STAR-CCM+ in a wide range of areas, such as investigating non-Newtonian fluid flow in evaporation, minimizing the loss of pressure in falling film evaporators, optimizing the separation efficiency in separators, optimizing the air flow in a spray dryer, and analyzing the recovery of waste heat at the dryer outlet.

Spray dryer: the goal is dry milk

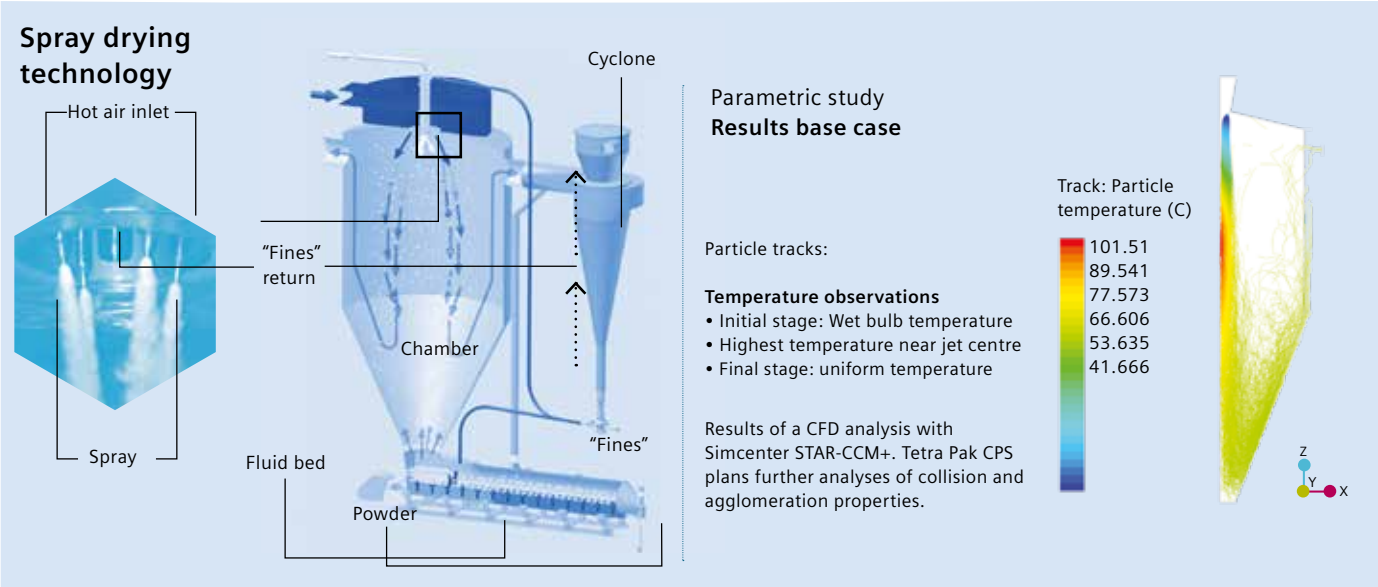
The spray dryer is based on the principle of surface enlargement, in which liquid products, such as milk or whey, are atomized into fine droplets through a flow of hot air, in which temperature ranges between 150 and 250°C. The droplets, which are dried as they fall, are only exposed to the airflow for 0.5 to 1 second.

The operator can only achieve a high-quality solid product retaining a small particle size with the smallest possible droplet size distribution. The size of the spray dryer depends on the drying time (fall time) and the desired size of the droplet/particle. This has resulted in impressive dimensions, as Jongsma describes: "A typical spray dryer has a volume of 700 m³ (diameter: 8.5 m; height: 20 m), processing 5T milk or whey an hour and using 5 MW of power. The energy efficiency lies between 40 and 65 percent – that makes every step towards optimization worthwhile!" The significant parameters of a spray dryer are:

- The chemical composition and the initial concentration
- The temperature of the hot air flow
- The mixing properties of the droplets and air
- The flight path and the agglomeration properties

Low-output spray dryer 1,000 per hour (kg/h). Typical plants have an output of 5 MW and a throughput of 5 t/h.

Tetra Pak CPS:
Tetra Pak Cheese and Powder Systems specializes in cheese making equipment and provides proven solutions for evaporated and dried powder technologies. Tetra Pak CPS is part of Tetra Pak, the world's leading food processing and packaging solutions company. Working closely with our customers and suppliers, we provide safe, innovative and environmentally sound products that each day meet the needs of hundreds of millions of people in more than 170 countries around the world. With almost 22,000 employees based in over 85 countries, we believe in responsible industry leadership and a sustainable approach to business. Our motto, "PROTECTS WHAT'S GOOD™," reflects our vision to make food safe and available, everywhere.



Spray dryer design.

The quality of a simulation relies on the accuracy of the underlying model – how realistic the relevant physical, chemical and technical processes are numerically described. In addition, to ensure a quick turn around, the simulation setup and execution should be easy, intuitive and efficient. Simcenter STAR-CCM+, with its unrivaled meshing technology, high-fidelity physics and user-friendly interface, meets all these requirements. Jongsma confirms that promise and reality match very well, noting, "I could not put a scale to it, but I can say I am very satisfied with the package itself, the workflow and the support that is given. There are of course limitations in what one can describe (in terms of physics) through CFD at the moment, but I see a steady growth in Simcenter STAR-CCM+ capabilities. These are made possible by the research efforts of numerous institutes around the world and it seems that this trend is not coming to an end any time soon." Jongsma continues: "In general terms, I can state that by actively using CFD we have greatly improved our understanding of the complex physics in spray dryers. We now know more about the conditions that are favorable for spray dryer operation. The objective here was to optimize the spray dryer output and minimize fouling. Fouling limits the running time of a spray dryer; after several weeks it needs to be cleaned. It appeared that the factors that minimize fouling also favorably affect the capacity. The factors that were optimized are the air flow into the system and the way the liquid is introduced (by high-pressure spray nozzles)." The benefits to the customer can be clearly defined: improved production capacity, powder quality and a longer period of time between necessary cleaning of the spray dryer.

The tool: Simcenter STAR-CCM+

Simcenter STAR-CCM+ provides a comprehensive engineering simulation inside a single integrated package. Much more than just a CFD solver, Simcenter STAR-CCM+ is an entire engineering process for solving problems involving flow (of fluids or solids), heat transfer and stress. Although this might sound complicated, it is actually very functional and easy to learn, confirms Jongsma: "It is demonstrated time and again: even on the basis of relatively simple models, computer-controlled simulation leads to astonishing results. The unique way in which Simcenter STAR-CCM+ is set up means the learning curve is really short. Creating a mesh, performing the simulation, and analyzing the results take place in a single interface. The fact that postprocessing can be carried out while the simulation is running is very helpful in reaching a converged solution."

Achieving better layer control in multi-layer polyester films with simulation

Introduction

What do books, circuit boards, solar panels, fresh and frozen foods and a driver's license have in common? It is something that has permeated our daily lives to such an extent that we barely stop to acknowledge its existence. The answer is polyester films - one of the most versatile and useful innovations of the last century. Polyester films find use in various applications ranging from photovoltaics, packaging, construction, health care, imaging and electronics. The company DuPont Teijin Films (DTF) has been at the forefront of bringing this multi-faceted product to the masses starting with its revolutionary research in the 1920s and 1930s, leading to the discovery and development of nylon and polyester films. Today, DTF is the world's leading producer of plain polyethylene terephthalate (PET) and polyethylene naphthalate (PEN) polyester films, constantly driving product and process innovation for polyester films.

This article is a summary of how DTF is using numerical simulation for layer configuration and control of multi-layered films (MLFs), the results of which will be directly transferable to production scale plants. DTF has teamed up with The Department. of Chemical Engineering at the University of Birmingham to use numerical simulation to gain further understanding of the coextrusion process used to produce MLFs. An MLF is formed when different polymer melt layers come together for the first time in either: i) an injector block linked to an end fed die or ii) a multi-manifold die (MMD). The Engineering and Physical Sciences Research Council (EPSRC) has sponsored this research due to its wide-reaching implications and benefits to the industry.

Polyester film production

In general, polyester films are manufactured with an extrusion process in which the polymers are extruded onto a cooling casting drum to make the polymer film, which is then stretched using a drawing process. The film is then crystallized under tension at high temperatures to obtain the final shape and molecular orientation. Polyester-based MLFs form a major part of DTF's product portfolio. MLFs are formed when different polyester melts, a polymer liquid above its glass/crystallization temperature, come together in a coextrusion process. MLFs are used in reflector films, data storage, cards and photovoltaic cells. At DTF, contrasting polymer melt layers form a single MLF structure in either an injector block linked to a die or a MMD. In the injector block, the melts are combined before being spread across the die whilst in the MMD, the melts are combined after being spread. Typical MLF structures produced by DTF are shown in figure 1, where A, B or C represent separate polymer layers in the MLF.

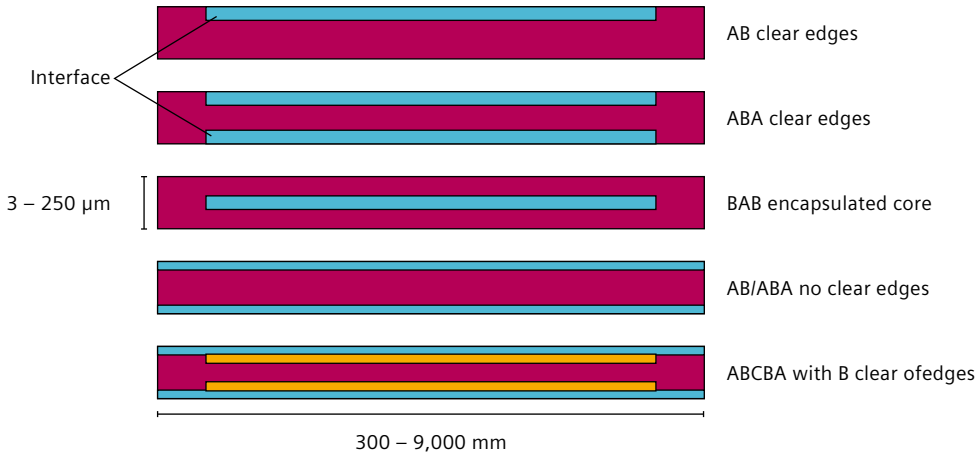


Figure 1: Typical MLF structure.

The key criterion during processing of such MLFs is the spreading across the die. The film is then cooled and stretched in both the forward and transverse directions to form the final polyester film. MLFs are typically 3-250 µm thick and around 300-9,000 millimeters (mm) long.

In a typical production process, the edges are trimmed before distribution, and trimming of thinner secondary layers is usually more expensive. The secondary layers can also contaminate the trimming clips leading to expensive repairs. Hence, it is desirable to have clear primary layer edges at the ends (known within the industry as clear edges). With a wide variety of melt layer thicknesses and melt flow properties, controlling the width and thickness of individual melt layers and the edges is becoming increasingly difficult and the key is proper layer control, increasing product performance and reducing expensive experiments.

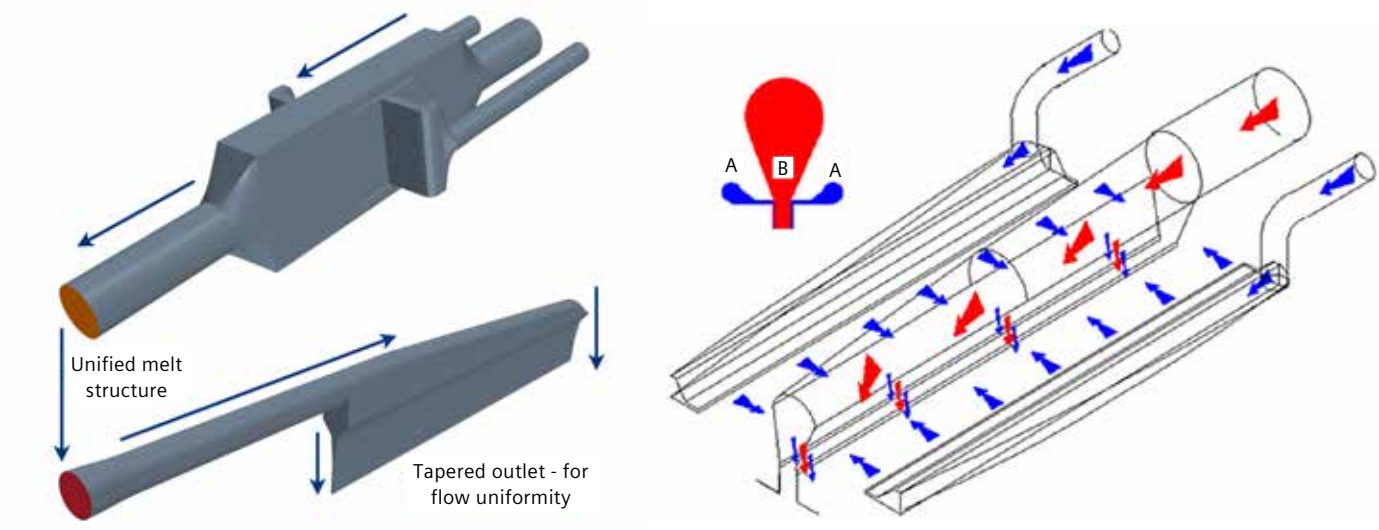


Figure 2: Common DTF coextrusion structures: injector block and end fed die (top) and multi-manifold die (bottom).

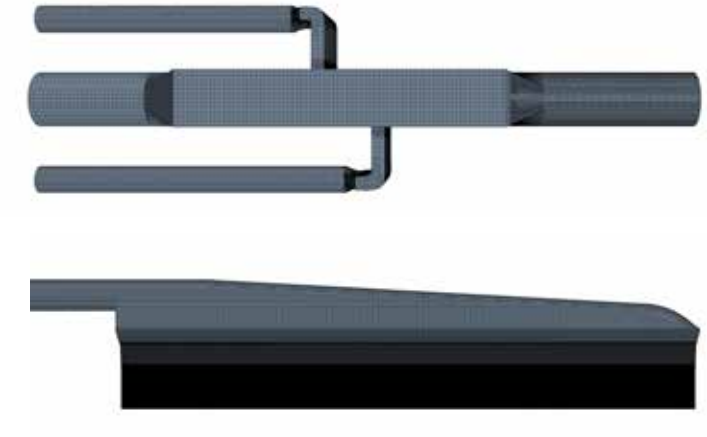


Figure 3: Mesh on the injector block and end fed die.

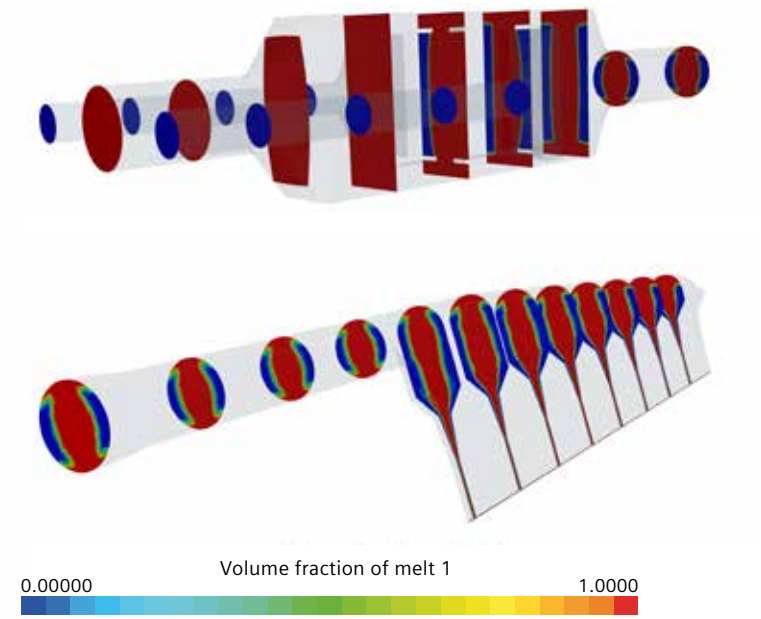


Figure 4: Progressive volume fraction at sections: injector block (top) and end fed die (below).

CFD modeling – end fed die

The two coextrusion structures used at DTF are shown in the image below. In the first case, the polymer melts are fed into the injector block and the unified melt structure comes out through a tapered outlet for flow uniformity and uniform final film structure. In the MMD, the primary layer enters the main block and the secondary layers enter through the side channels with the unified melt exiting through a tapered die outlet. A comparative computational study of the two coextrusion processes used at DTF is presented here. Simcenter STAR-CCM+ was chosen as the preferred simulation platform after evaluating different computational tools for this purpose.

Firstly, an Eulerian Multiphase (EMP) simulation of the coextrusion process in the injector block and end fed die was conducted. The volume of fluid (VOF) capability of Simcenter STAR-CCM+ was used to model and track the interface between the different polymer melts, and the EMP model allows seamless simulation of two or more phases. The flow was assumed to be laminar, Newtonian and incompressible. The two melts were initially identical in nature, with the later simulations having increased viscosity of the secondary melt. The domain was discretized using trimmed hexahedral cells in Simcenter STAR-CCM+. The injector block contained 1.5 million (M) volumetric cells, while the end fed die contained 14.5 M cells. The two melts were initialized with a temperature of 285° C, density of 1,250 kg/m3, melt viscosity of 170 Pa-s and a thermal conductivity of 0.2 W/m/K. The mass flow

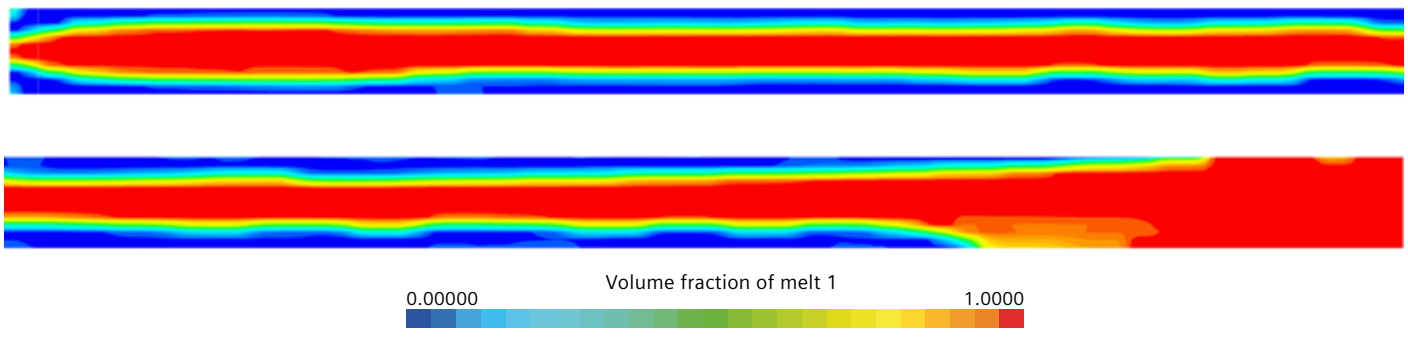


Figure 5: Volume fraction at outlet for injector block and end fed die.

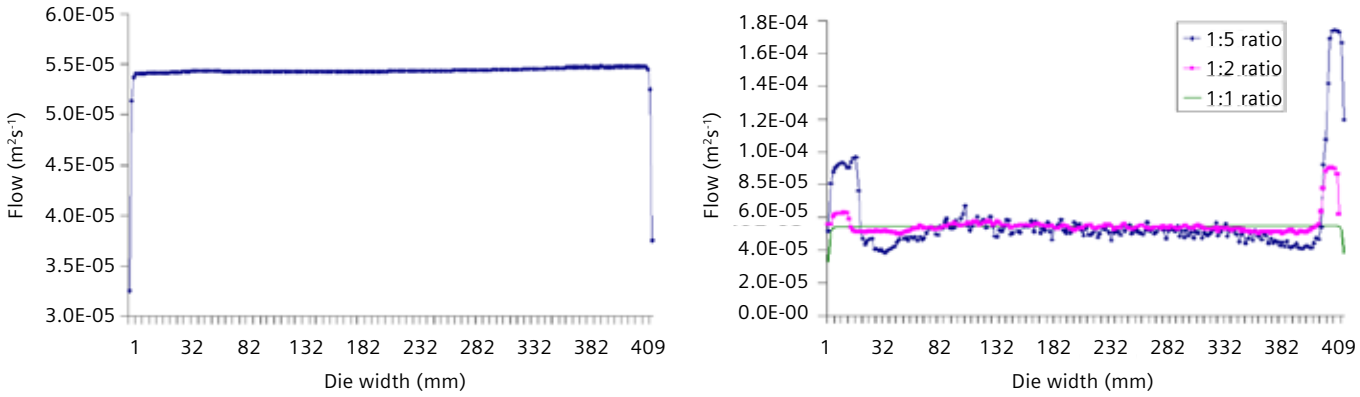


Figure 6: Flow across the outlet for 1:1 viscosity ratio (left) and flow across outlet for increasing ratios (right).

Figure 7: Mesh on multi-manifold die (MMD).

Viscosity (Melt 1:Melt 2, Pa s)	Blank end, air side clear edge width (mm)	Flow difference (percent)
170:170	7.2	0.73
170:340	7.2	4.14
170:850	9.8	9.56

Table 1: Flow difference at outlet.

Viscosity (Melt 1:Melt 2, Pa s)	Clear edge width (mm)	Flow difference (percent)
170:170	11.0	5.04
170:340	10.9	3.11
170:850	10.7	2.66
170:850	10.1	2.18
170:1,700	9.7	2.00

Table 2: Flow difference at outlet for MMD.

rate of the primary melt 1 was 80 kilograms per hour (kg/hr) and the secondary melt 2 was 20 kg/hr, leading to corresponding volume fractions of 80 percent and 20 percent respectively. All simulations were run on a Dell Precision workstation, with a 32 gigabyte (GB) memory.

The image below shows the progressive volume fraction of the melts through the injector block and end fed die. The unified melt structure at the outlet is of type ABA with melt 1 in red at the center flanked by melt 2 in blue on either side. The progressive volume fraction plot shows that the ABA structure is maintained with a smooth interface in both the injector block and end fed die. The injector block geometry is asymmetrical with the left side melt 2 entering before the right side melt 2. The second image shows the outlet volume fraction in the end fed die. The simulations show that clear edges are not present with either melt 2 layer at the 0 mm edge. This is despite experimental work suggesting the presence of clear edges. The lack of clear edges in the simulation can be attributed to the transition region from horizontal to vertical flow in the die not being properly resolved with a finer mesh. The top melt 2 layer has spread wider than the bottom melt 2 layer at the 410 mm edge in the simulations (figure 5). A uniform final thickness is produced at the end fed die outlet. Plots of flow rate across the width of the outlet show very small flow difference, suggesting uniform final thickness due to the wide taper (figure 6).

Simulations were also carried out by increasing the viscosity of the secondary melt layers to 2 and 5 times the viscosity of the primary melt layer. The plot of flow across the width of the outlet for the three cases (figure 6) shows that as the viscosity of the second layer is increased, there is less flow uniformity across the outlet, suggesting a final melt layer of decreased uniformity. The accompanying table lists the clear edge width at the 410 mm end of the end fed die outlet and the flow difference across the outlet width for all melt ratios.

CFD modeling of a multi-manifold die

Similar to the modeling of the injector block and end fed die, simulations were carried out based on the MMD concept to compare the final layer structure and thickness. A trimmed hexahedral element mesh with 12 million volumetric cells was created with enough refinement along the tapered end as shown in the image. Simulations were carried out with the same conditions as the injector block and end fed die. Contour plots of the progressive volume fraction through the MMD show the formation of an ABA structure with smooth interfaces between the melt layers. Velocity vectors of the flow field show the effect of melt 2 entering for the first time, causing deformation of melt 1. The outlet volume fraction plots show the structure of the final unified film, which is more uniform compared to the end fed die. The flow is more symmetrical in the MMD and there are clear edges of equal width on either side. Thus, the MMD is better for processing due to

Numerical simulation helps the user understand the coextrusion process of polyester films and how clear edges are obtained. The benefits include easier processing and reduced processing cost with clear edges.

the uniform nature of the secondary melt 2 layers in the final film and the presence of clear edges on both sides of the outlet. The viscosity of the secondary layers was increased correspondingly to 2, 3, 5 and 10 times that of the primary layer viscosity. Simulations show that across the width of the outlet, the core part of the unified structure is linear and uniformly thick while the edges show extreme peaks, with only the less viscous primary melt 1 layer present. The decreasing flow difference at increased secondary layer viscosities suggests the MMD is better for structures with larger secondary layer viscosities and more efficient computationally.

Conclusion

Comparison of numerical simulations of multi-layered polyester film formation through both an injector block linked to an end fed die and a MMD shows that clearer edges are obtained from the MMD,, which is beneficial in production. In addition, the MMD produced a more uniformly thin final film and a smoother melt interface with wider viscosity ratios. Numerical simulation will be highly beneficial if extended to wider, industrial-scale geometries to clearly understand the coextrusion process of polyester films and how clearer edges are obtained. Simulation can also throw light on the impact of secondary layers with smaller viscosities on the polyester based MLF formation. The benefits include easier processing and reduced processing cost with clear edges.

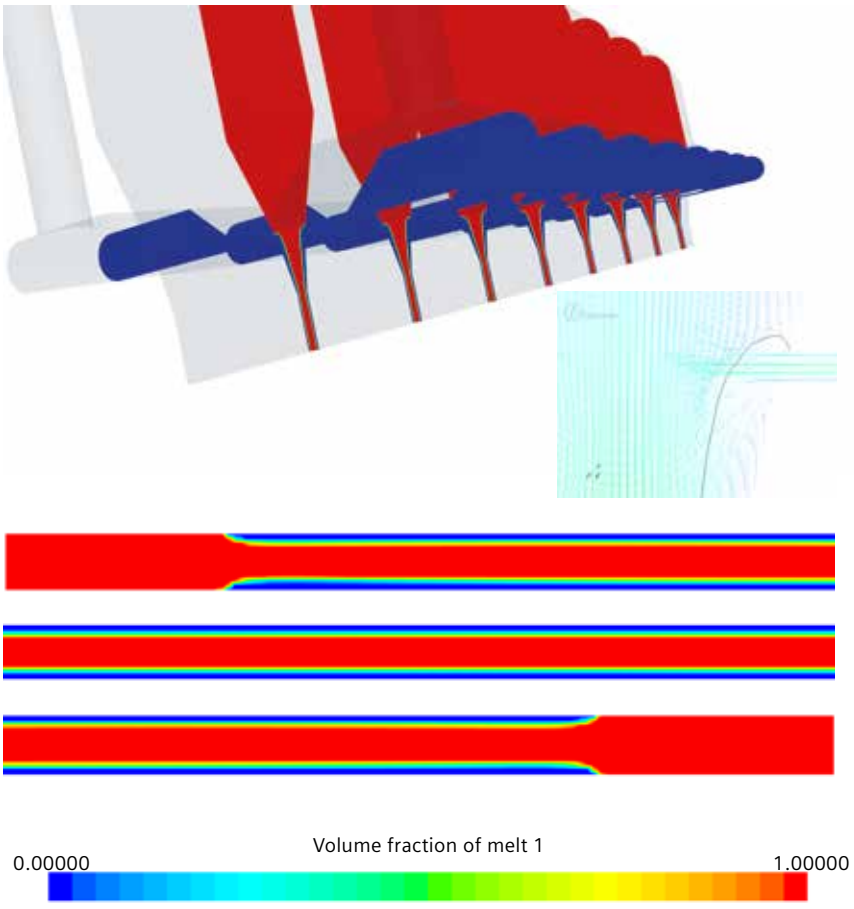


Figure 8: Progressive volume fraction (top) and outlet volume fraction (bottom) in MMD.

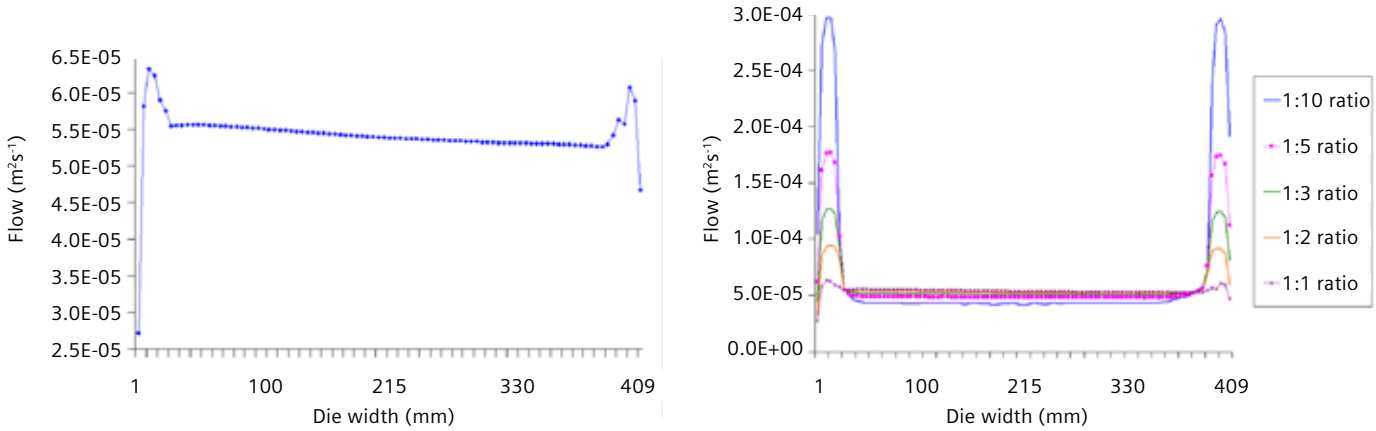


Figure 9: Flow across the outlet for 1:1 viscosity ratio (left) and flow across outlet for increasing ratios (right) for MMD.

Numerical simulations for continuous manufacturing of active pharmaceutical ingredients

With unprecedented economic pressures and increased global competition, pharmaceutical manufacturing companies are continuously looking to gain a competitive advantage by improving the efficiency of their processes and the quality of their products. Traditional manufacturing processes, which are batch processes, are no longer sustainable and there is no question that continuous manufacturing is the clear path forward towards leaner processes. Multi-physics numerical simulation is emerging as a game-changing technology to help continuous manufacturing for active pharmaceutical ingredients (APIs) become a reality with virtual prototyping, optimization and modeling of the complete system.

From batch to continuous processing

The pharmaceutical industry is encountering a decline in productivity, and outdated tried-and-true batch processes are at the root of the problem. The batch-based systems currently in place are inefficient due to segmented steps involving multiple facilities and requiring start-and-stop of the batch, site-to-site transfer and warehouse storage. Performed with sampling and in post-production, quality assessment of the product is also cumbersome, causing long lead times and waste.

Continuous manufacturing, a nonstop end-to-end manufacturing process, could modernize the industry and solve its productivity crisis. At a recent Massachusetts Institute of Technology (MIT) conference, Josef Jimenez, chief executive officer (CEO) of Novartis, stated that changing production from batch to continuous will transform the way medicines are made around the world and could cut the time from development to market entry in half [1]. Implementation of these processes will result in smaller production plants, lower inventory costs, a reduced carbon footprint and higher quality products [2].

The regulatory agencies are also starting to lay the groundwork for continuous manufacturing with several initiatives [3, 4], and regulatory frameworks such as the Process Analytical Technology (PAT) and Quality by Design (QbD). Each of these encourages the development of new manufacturing technologies by building quality into the process and using a science-based quantified risk approach.

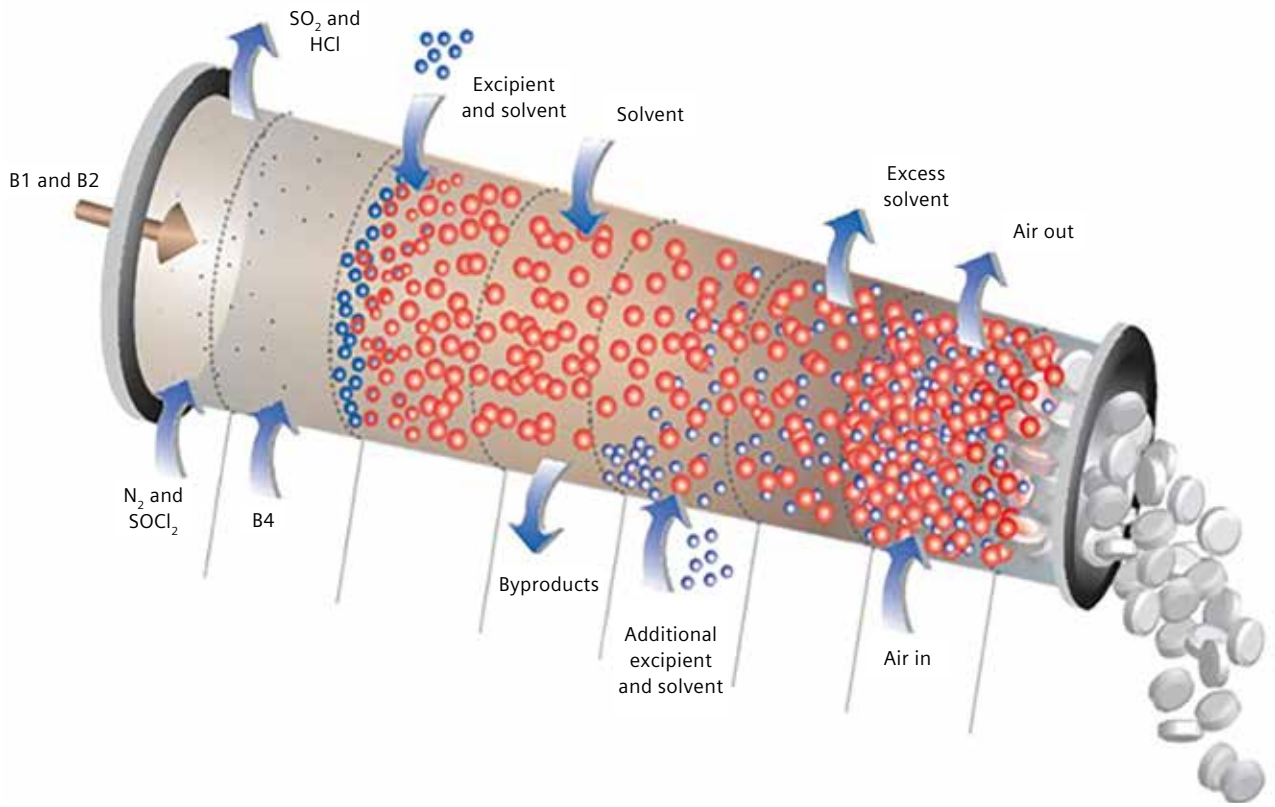


Figure 1: Ultra-lean manufacturing, from start of chemical synthesis to final pharmaceutical dosage form (courtesy of Novartis-MIT Center for Continuous Manufacturing).

Both the chemical and food processing industries have been improving their productivity by successfully integrating continuous manufacturing into their plants. It is clear that regulatory hurdles and conservative thinking by the pharmaceutical industry can no longer be used as an excuse to avoid taking pharmaceutical manufacturing into the 21st century.

Numerical simulations and continuous manufacturing

Before continuous manufacturing can become mainstream, potentially suitable candidate processes must be identified and designed, and risks must be analyzed and mitigated. This will help manage regulatory compliance and make a business case for implementation. Multi-physics computational fluid dynamics (CFD), a numerical method for predicting the coupled behavior of fluid, gas and particulate flow,s including heat and mass transport, offers a solution for the enhanced understanding and design of these novel processes.

Virtual prototyping

Traditional manufacturing processes are based on the "design-build-test" principle in which the effects of design changes are quantified by experimental tests on physical prototypes. There are currently very few suppliers who are developing integrated systems for continuous manufacturing and, as a result, physical prototyping is anticipated to be very costly. Numerical simulations enable the engineer to build a virtual laboratory, providing insight into the performance of a product before tests are carried out. This means the uncertainty resulting from major process and equipment changes can be evaluated up front, leading to a significant risk reduction and cost savings.

Multi-physics CFD and state-of-the-art visualization tools also offer a wealth of detailed information, not always readily available from laboratory or experimental tests. This not only results in an increased level of insight into the details of what is going on inside the

Case study one:
Direct element modeling (DEM) for pill coating

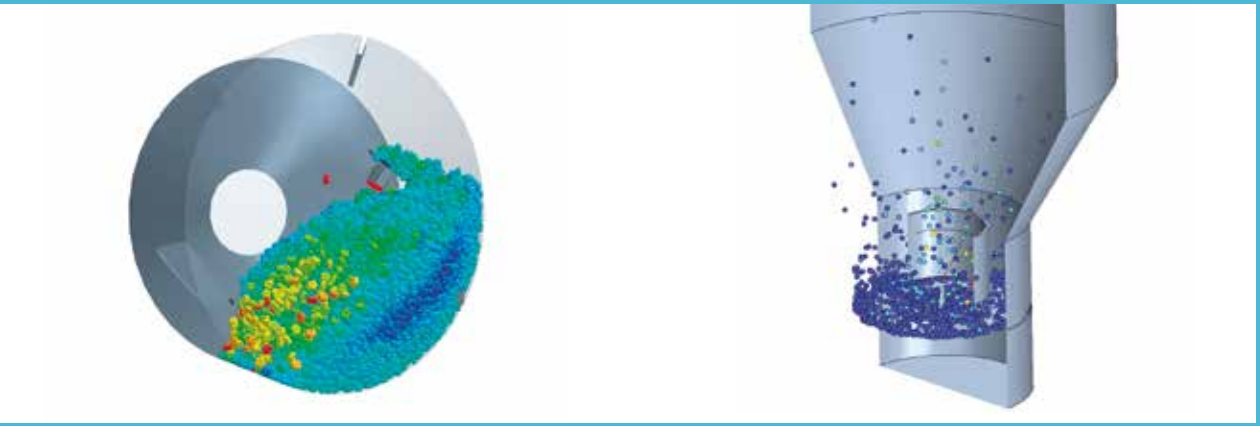


Figure 2: DEM simulation with Simcenter STAR-CCM+ showing tablet velocity magnitude as they tumble in a coating pan.

Figure 3: DEM simulation for tablet coating with Simcenter STAR-CCM+ showing pill coating thickness in a fluidized bed.

DEM simulates the motion of a large number of interacting particles and tracks them in a numerically efficient manner, modeling contact forces and energy transfer due to collision and heat transfer between particles. DEM will be particularly important in the design and optimization of continuous coating processes to help identify the important factors for equipment design (for example number of spray guns) and to determine optimal equipment operation conditions (for example inlet temperature).

Figures 2 and 3 show Simcenter STAR-CCM+ generated solutions for two types of equipment currently used for real-world tablet coating: coating pan (rotating drum) and fluidized bed. In these simulations, DEM is used to analyze the random movement of the particles as layers of coating are applied. Parameters such as particle velocities, residence time and coating thickness are tracked to assess and improve tablet coating uniformity. In addition to tablet coating, DEM can also be used to simulate other steps in manufacturing such as filling, filtering and conveyer processes.

processes but also enables innovation. For example, multi-physics CFD can help explore new reactions and molecules for drugs manufactured with a continuous process.

Design exploration and optimization

In recent years, the phenomenal increase in computing power and the maturing of robust simulation tools have paved the way for using numerical design optimization in production environments. Parameter studies and optimization will be vitally important for designing and tuning of the new (often smaller) equipment required for continuous manufacturing while ensuring the operation can efficiently handle fast reactions and remains flexible.

In addition, the CFD-generated responses – obtained with design of experiments over a range of operating conditions and equipment design parameters – can be combined with statistical models to identify risk and implement robust real-time process control. This will ultimately result in reduced variability and consistent, repeatable processes. Optimate™ (a module in Simcenter STAR-CCM+ using HEEDS™ software) is an example of a tool that enables intelligent design exploration to easily consider what-if scenarios and identify the critical manufacturing points that define quality. For example, feeding devices for continuous manufacturing influence all downstream operations and design exploration of parameters, such as feed rate, will help identify their impact on final blend uniformity.

Simulating the system

Solving complex real-world problems demands an accurate, easy-to-use, multidisciplinary approach to simulating complete systems. CFD-focused multi-physics engineering simulation tools such as Simcenter STAR-CCM+ can be used to accurately deliver full spectrum engineering results and the pharmaceutical industry should fully leverage these tools in support of the development of continuous manufacturing processes. Up until now, integration of numerical simulations in a production environment has required a great deal of specialized knowledge, but this is no longer a showstopper. Automation and ease-of-use are enabling the deployment of CFD for complex multi-physics applications.

For example, Simcenter STAR-CCM+ offers state-of-the-art meshing, seamless integration with CAD and easy modeling of complex moving parts, all in a single integrated

Case study two:
Eulerian multiphase (EMP) modeling for mixing

Figure 4: Mixer model showing the effects of increasing gas injection rate using Simcenter STAR-CCM+.

EMP modeling provides an effective means for studying the interacting streams and randomly dispersed phases in multiphase flows. The EMP model in Simcenter STAR-CCM+ includes an extensive range of sub models such as break-up and coalescence models for bubbles and droplets, and a granular flow model for particles. Figure 4 demonstrates an EMP simulation of a gas-liquid mixer with three rotating impellers. Shown are the effects of increasing gas injection rates on gas. The ability to predict gas hold-up, a parameter that governs mass transfer across the phases and consequently rates of reaction, is a key enabler in the design of such reactors. This approach adds valuable scientific insight into the decision-making criteria to develop practical solutions for mixing and other processes in continuous manufacturing.

environment. The net result is more time for an engineer to analyze data instead of preparing and setting up the simulations, resulting in engineering success. Seeing the big picture for continuous manufacturing will require a multi-physics approach to solving problems. Be it mixing, coating or drying, multiphase flows lie at the core of the pharmaceutical processing industry. Capabilities such as discrete element modeling (DEM), a numerical method for computing the interaction of a large number of small particles, and Eulerian multiphase modeling (EMP), a numerical method for simulating several phases in a system, will be invaluable for implementing continuous manufacturing of application programming interfaces (APIs). The two case studies in the article nicely demonstrate these capabilities.

Conclusion

In today's competitive climate, manufacturing must become leaner with a focus on building quality into the process. Continuous manufacturing for the pharmaceutical industry will change the way drugs are made and multi-physics CFD simulations offer a cost-effective way to perform rapid prototyping for design of new equipment and processes. In particular, design optimization tools and powerful multiphase models such as DEM and EMP will play an important role, and the pharmaceutical industry should fully leverage these future state-of-the-art technologies for the design and implementation of continuous manufacturing processes.

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3. "The FDA Critical Path Initiative and its Influence on New Drug Development," Woodcock J., Woosley, R. , Annu. Rev. Med. 2008. 59:1–12.
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Numerical simulations for tableting and coating

Solid dose tablet manufacturing processes often lack reliability and robustness as a result of errors in production and a shortfall in process control. Facing unprecedented economic pressures, pharmaceutical manufacturing companies are continuously looking to improve on the quality of their products and the productivity of their processes. Multi-physics numerical simulation is emerging as a game-changing technology to help step up efficiency, enhance quality and shorten time-to-market through virtual prototyping and optimization.

Challenges of solid dose tablet manufacturing

Tableting (compression from a powder into a solid dose tablet) and tablet coating are two vitally important steps in the tablet manufacturing process that ultimately determine the weight, thickness, density, hardness and coating of the final solid dosage form. Variability in any of these attributes not only negatively impacts the release profile and therapeutic efficacy of the medicine, it alters the disintegration and dissolution properties of the tablet, leads to tablet defects and causes breakage during bulk packaging and transport.

With the adoption of novel manufacturing processes such as nonstop end-to-end processing, and the push to build quality and efficiency into production, solid dose tablet manufacturers have a challenging road ahead of them because they must pinpoint the key factors and requirements that will lead to robust and repeatable processes, resulting in superior products.

Why numerical simulations?

Multi-physics computational fluid dynamics (CFD) is a numerical method for predicting the coupled behavior of fluid, gas and particulate flows including heat and mass transport. A significant advantage of using numerical simulations is that it allows for the validation of a design or process before physical tests need to be carried out. For example, the development of a new tablet shape or coating material calls for performing an extensive number of costly and time-consuming experiments to avoid unexpected variations, identify unpredictable process parameters and address scale-up problems. Studying these effects using numerical simulations can greatly reduce time, material and development costs. In addition, numerical visualization tools offer a wealth of detailed information, not always readily available from experimental tests. This not only results in an increased level of insight into the details of what is going on inside the processes, it enables innovation.

Simcenter STAR-CCM+ provides the solutions

With its automated polyhedral meshing technology and comprehensive range of physics models, Simcenter™ STAR-CCM+™ software is a complete multidisciplinary simulation toolkit to tackle a wide range of applications in the pharmaceutical industry. One capability in Simcenter STAR-CCM+ that is particularly well-suited for the simulation of tablet manufacturing processes is discrete element modeling (DEM), which is fully coupled with numerical flow simulations and delivered in a single software environment.

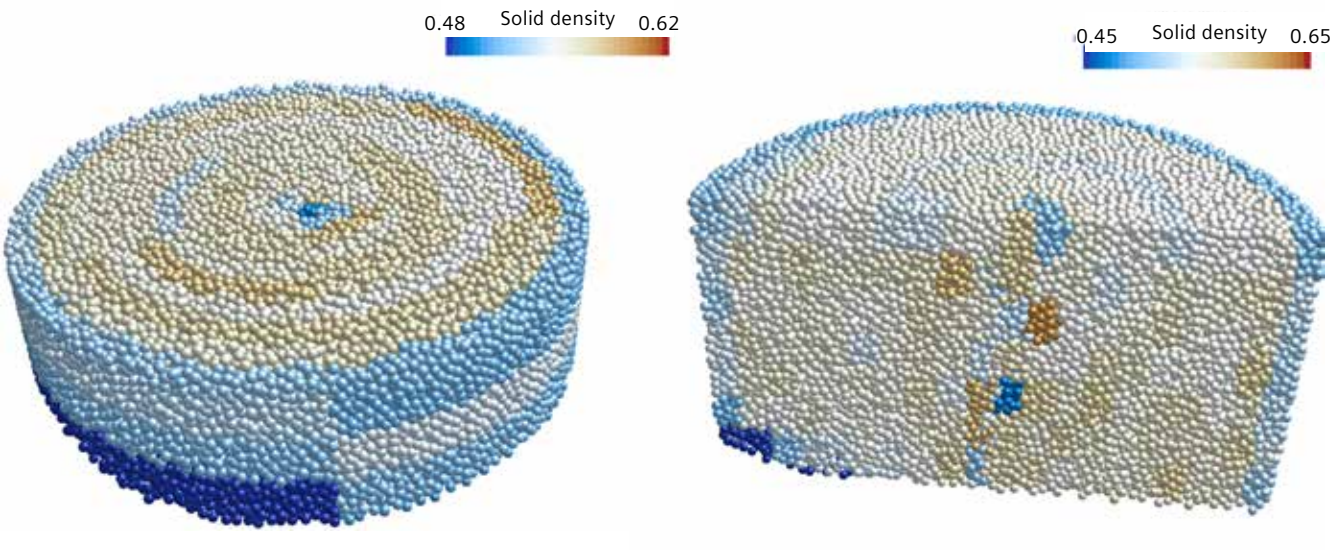


Figure 1: Simcenter STAR-CCM+ simulation with DEM showing a pharmaceutical powder packed and compressed inside a tablet die. Variations in color reflect the nonuniformity of the granule distribution.

Tableting and coating involve a large number of discrete particles that interact with each other and the fluids surrounding them. DEM accurately tracks these interactions and models contact forces and energy transfer due to collision and heat transfer between particles and fluids. The DEM capability in Simcenter STAR-CCM+ can predict dense particle flows with more than one million particles in a reasonable time, making it practical for analyzing real-world tablet manufacturing processes such as filling, compressing/compacting, coating and drying.

Figure 1 shows the results obtained from a Simcenter STAR-CCM+ simulation of precompression in a tablet press to determine how to overcome common tablet defects such as capping, (splitting of the tablet's upper cap) which often occur as a result of entrapment of air and migration of fine particles during the compression process. DEM is used to track the interaction of the particles with each other and with the die as they are rearranged and moved into the empty spaces during precompression. This simulation offers a detailed look at the uniformity of the granule distribution and can help determine the optimal precompression force and dwell time required to ensure that fine particles will be locked in place before compression starts, greatly reducing the risk of incurring common tablet defects during production.

DEM simulations with particle-fluid interactions also provide realistic solutions to assess the uniformity of film coating thickness, a critical parameter for tablet quality. Figure 2 depicts a simulation performed with Simcenter STAR-CCM+ for the coating process in a fluidized bed where DEM is used to analyze the random movement of particles as their trajectories change while layers of coating are applied. Parameters such as particle velocities, residence time and coating thickness are monitored during the simulation. These can be fed as objective functions into Optimate™, a module in Simcenter STAR-CCM+ that enables intelligent design, to help identify the important factors for equipment design (for example nozzle spacing) and to determine optimal equipment operating conditions.

Simcenter STAR-CCM+ also has a novel Lagrangian passive scalar capability, enabling the user to easily monitor the coating thickness and other features of tablets. Figure 3 illustrates a case in which more than 70,000 tablets are tumbled in an industrial coater. The goal of the study is to improve on interparticle coating uniformity by determining optimal spraying equipment settings in the tumbler. Two Lagrangian passive scalars representing coating thickness are defined: one with source volume confined to one cone above the surface, another with source

In today's competitive climate, manufacturing of solid dose tablets must have a focus on building quality and efficiency into the processes. This can be accomplished through rapid prototyping and optimization using multi-physics simulation.

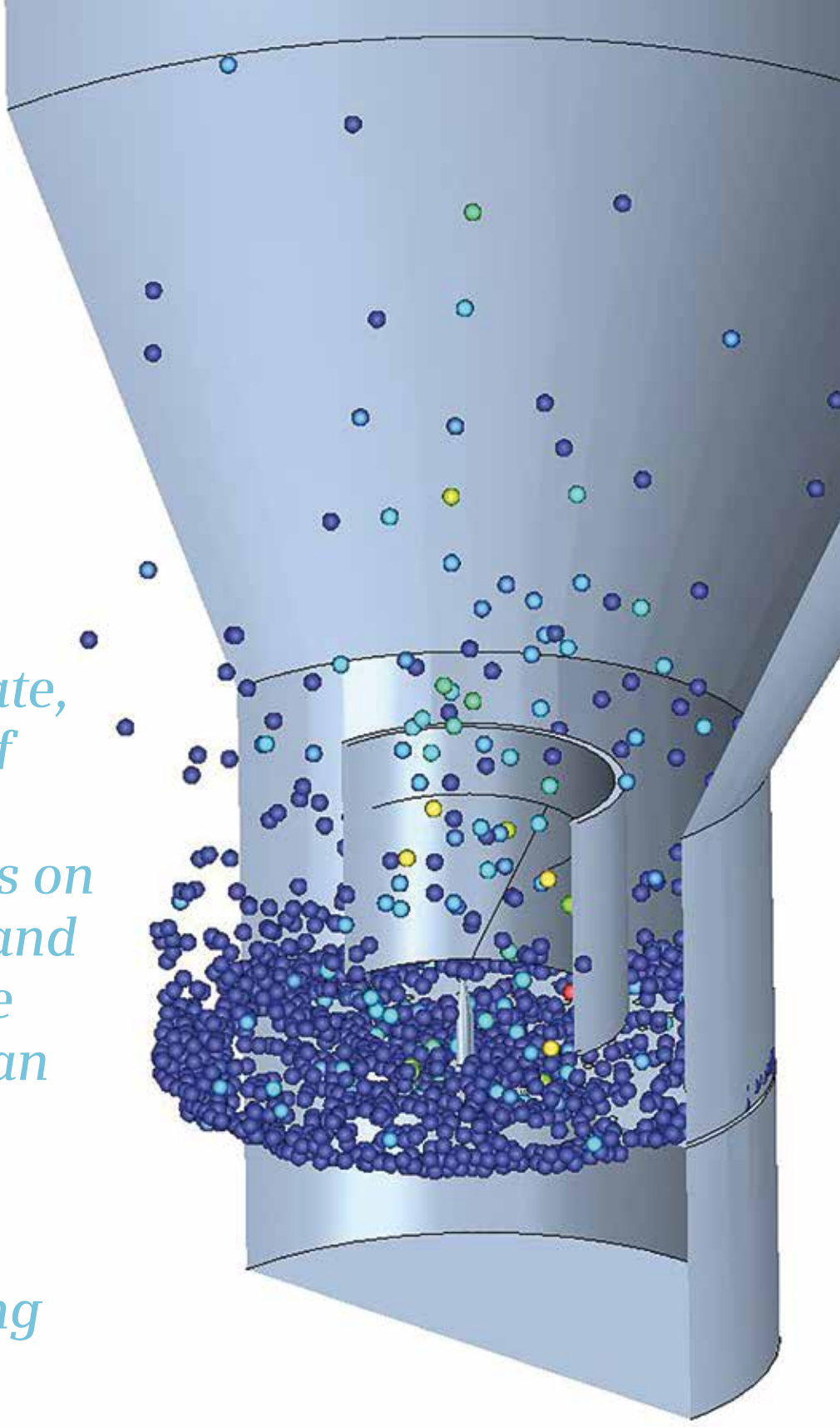
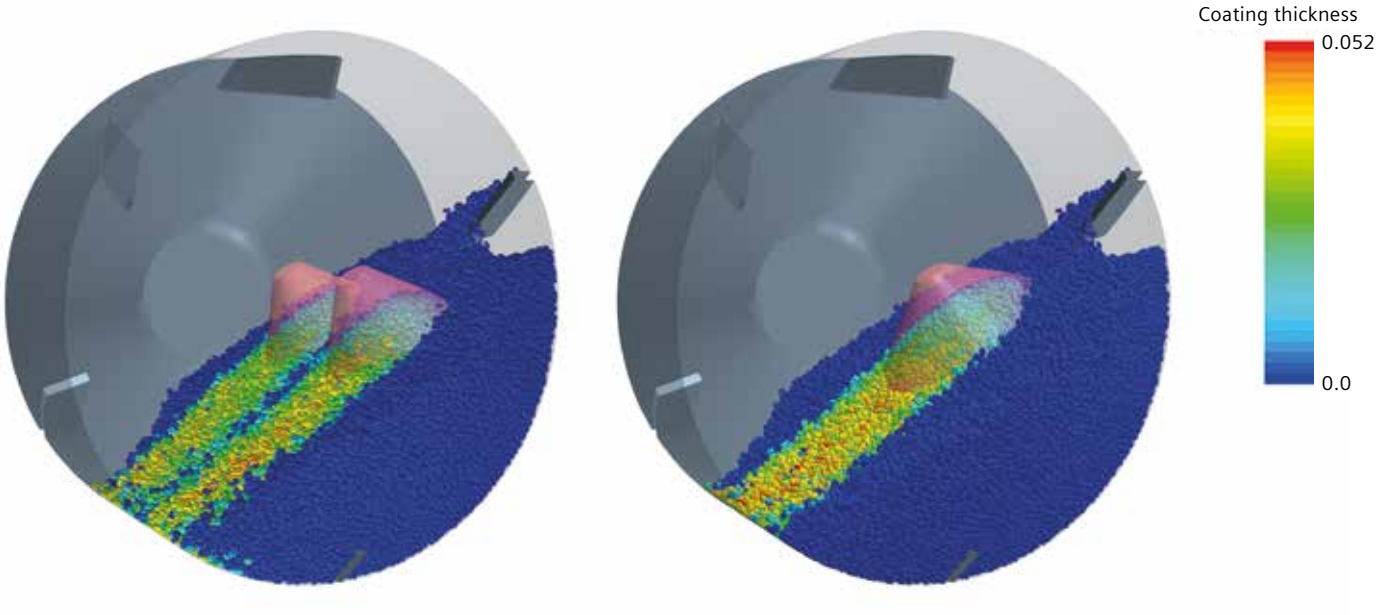


Figure 2: Simcenter STAR-CCM+ simulation of the coating process performed in a fluidized bed.



volume confined to two cones and with an effective spray area identical to the one of the first passive scalar. Using this approach, a single simulation allows for a comparison of the interparticle coating uniformity for two different spray zones and the result indicates the two-spray configuration provides a more uniform coating distribution.

Conclusion

In today's competitive climate, manufacturing of solid dose tablets must have a focus on building quality and efficiency into processes, and multi-physics CFD simulations offer a cost-effective way to achieve this through rapid prototyping and optimization.

The complex flow-fields associated with tableting and coating can be addressed with ease by using the high-end physics models delivered by Simcenter STAR-CCM+, including the powerful DEM and novel passive scalar capabilities. Users in the pharmaceutical industry are fully leveraging these state-of-the art technologies as it opens the door to explore innovative ways to improve quality, reduce cost and shorten time-to-market.

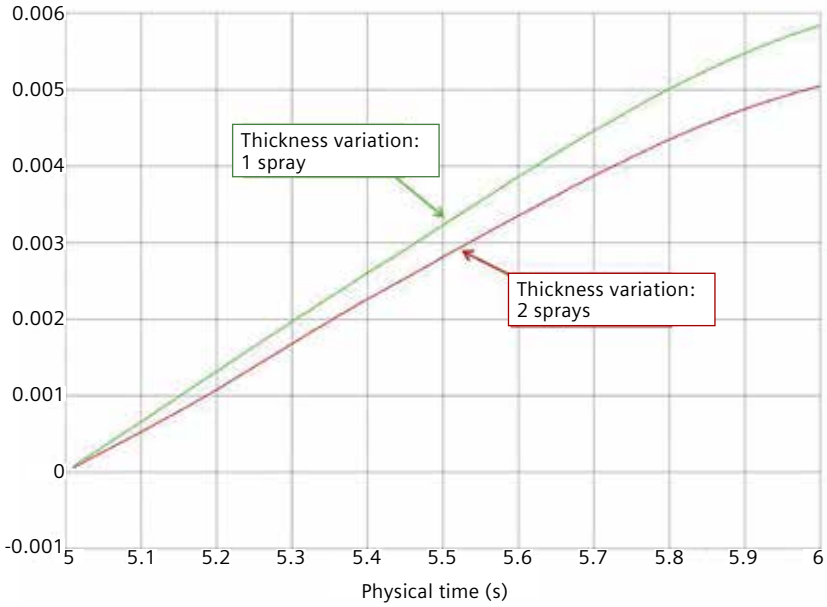


Figure 3: Simulation with Simcenter STAR-CCM+ comparing coating thickness variation of one and two sprays in a tumbler.

When CFD secures the manufacturing process of vaccines

Creaform was asked to assist in the design of a cleanroom by performing a complete 3D reconstruction of the geometry of the room, and using this to carry out detailed CFD simulations. The cleanroom in question is used in the manufacturing of influenza vaccine, and the aim of the study was to design an efficient aerodynamic barrier that would mitigate the risk of contamination. The demonstration was convincing and CFD simulations shed light on phenomena that traditional smoke tests, still used for regulatory compliance of pharmaceutical environments, had never been able to resolve before.

Introduction

The pharmaceutical cleanroom in this study is a critical environment requiring a high level of protection against contamination. While the cleanroom is a grade B environment, the interior of the restricted access barriers (RABS) is protected with screened barriers and HEPA high-efficiency particulate air (HEPA) clean-air filtration, so it is rated as a grade A critical zone. The vaccine filling machine had to be incorporated in the RABS, leading to many specific flow interactions that could not be predicted prior to installation, either by the manufacturer or the integrator.

It was therefore necessary to thoroughly understand the fluid flow behavior in order to ensure proper flow path around nonsterile components of the machine. Not only was the regulatory compliance of the cleanroom at stake, but with the amazing production rate of the line (hundreds of vial fillings per minute), a contamination would represent a considerable financial loss because it would lead to wasted of vaccine doses. In that context, Creaform's 3D modeling and computational fluid dynamics (CFD) solutions came in very handy. Using basic STL files such as the ones created by 3D scanners, the engineering team numerically reproduced the cleanroom in computer-aided design (CAD) software and performed a series of CFD simulations using Simcenter STAR-CCM+.

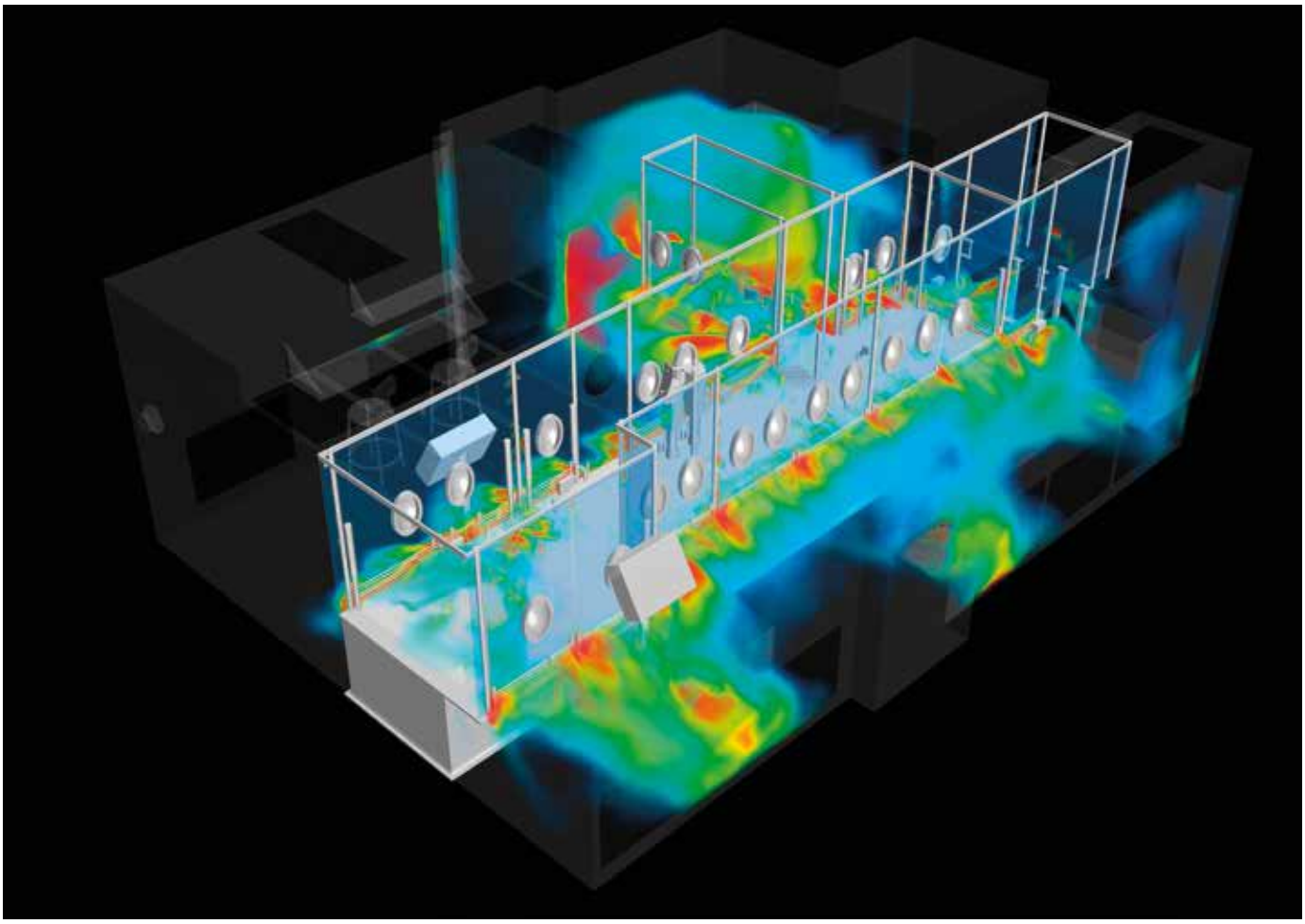
The stakeholders

Creaform

Creaform's mission is to develop, manufacture and market cutting edge portable 3D measurement and analysis technologies that increase productivity. With its expertise and the passion and commitment of its employees, Creaform helps companies from the manufacturing industry to seamlessly create, simulate, verify and collaborate in 3D, significantly enhancing their turnaround times and profitability. With its 3D engineering services department, Creaform develops CFD simulation techniques in multiple fields like transport, energy, environment, civil works, electronics and heating, ventilation and air conditioning (HVAC). For the project discussed here, Creaform was responsible for the CAD reproduction of the entire pharmaceutical production line and surrounding cleanroom, the CFD simulation of the air flow with RABS and HVAC systems in operation, and the assessment of aerodynamic deflectors to optimize flow behavior around nonsterile components.

Laporte consultants Inc.

Laporte is a consulting firm that specializes in biopharmaceutical,, food and beverage and industrial engineering. Its employees have experience in a wide array of services in the process, building and infrastructure, automation, packaging and regulatory compliance fields. In the context of this



project, Laporte was in charge of the process design, installation and commissioning for the pharmaceutical facility upgrade. These tasks include the HVAC design and the integration of the filling machine in the RABS system. Laporte was also responsible for the preliminary smoke tests used for regulatory compliance.

Computational geometry

A typical headache when carrying out a CFD analysis is not having the geometry available. An even bigger headache is not having confidence in the numerical geometry because the as-built drawings are incomplete or the geometry has changed over time. This situation brings the engineers to constantly question the CFD results. Creaform, by supplying efficient 3D scanning solutions, ensures high quality numerical reproduction. Creaform also manufactures fast, portable and easy-to-use scanners that provide metrology grade accuracy and resolution. For CFD applications in the HVAC industry, it is quite common for Creaform's engineers to combine the scan of an entire room acquired by a midrange scanner with the precise scan of specific parts using one of Creaform's handheld scanners (see figure 2). The result is a clean STL file such as the one built for the pharmaceutical cleanroom.

The numerical geometry of the cleanroom includes the walls and furniture, the HEPA filtration, the HVAC system, the physical barrier with gloved access (windows surrounding the production line), the control panels as well as the RABS with the accumulation table for vials, the conveyor, the filling needles, the capping machine and many measurement instruments, all of which were accounted for in the CFD simulations thanks to the wrapping capabilities of Simcenter STAR-CCM+.

Figure 2: Room scan using Creaform's handheld MetraSCAN.

Simulations

Precise and representative boundary conditions are critical for the cleanroom simulation. They were carefully determined using very recent data acquisition:

- Laminar flow equipment performance evaluation providing air velocity profiles for each diffuser of the HEPA filtration system
- Ventilation balancing measurements for the HVAC system including return ducts
- Precise pressure measurement in adjacent rooms for secondary air flow rates through wall openings for conveyor and through the door contour.

Turbulence modeling was achieved with the RANS approach and more specifically with the SST (Menter) k-omega model, thus limiting the results to steady state. The All y+ Wall Treatment was used because many near wall cells fell within the buffer region of the boundary layer. The control over the entire surfaces to force viscous sublayer resolution was computationally expensive and judged unnecessary. Indeed, calculation of viscous forces is not required and flow separation occurs at cutting edges, so its prediction is trivial. Consequently, the mesh is polyhedral and does not make use of prism layers. The prioritized cell refinement was the one that captured the surface details of the machine components, resulting in a cell count of 5.6 million for initial runs (setup check and initial solution) and of 18.4 million for final runs. Simulations made use of the coupled flow model with a second order discretization.

Results

Overall pressure distribution

Ideal flow conditions just above the conveyor level consist of a perfectly vertical flow. Pressure distribution in the horizontal plane is thus very important and must be as uniform as possible inside the RABS. The first CFD simulation of the cleanroom showed a small pressure gradient that was sufficient to induce a longitudinal component to the velocity vectors inside the RABS. Laporte engineers designed deflectors to redistribute the pressure in the capping section and removed the partition that provoked a pressure increase in the vials accumulation section. Combined with the modular adjustment of the HEPA filtration, these modifications significantly improved the pressure distribution in the RABS (see figure 5). The CFD simulation correlates well with the smoke tests performed with the new design and confirmed the improvement efficiency.

Transverse flow

With the longitudinal flow corrected, Laporte and Creaform focused on transverse velocity components in the vicinity of nonsterile machine components. The CFD simulations highlighted two similar undesired situations: one around the needles holder and one around the capping arm. Both components are nonsterile and the air draft from underneath the physical barrier induces a significant transverse velocity component. As can be seen in figure 6 (a), this phenomenon drives particles in contact with the arm directly toward the vials that are conveyed at the level of the toothed plate. The

Figure 3: Hexahedral mesh of vials conveyor.

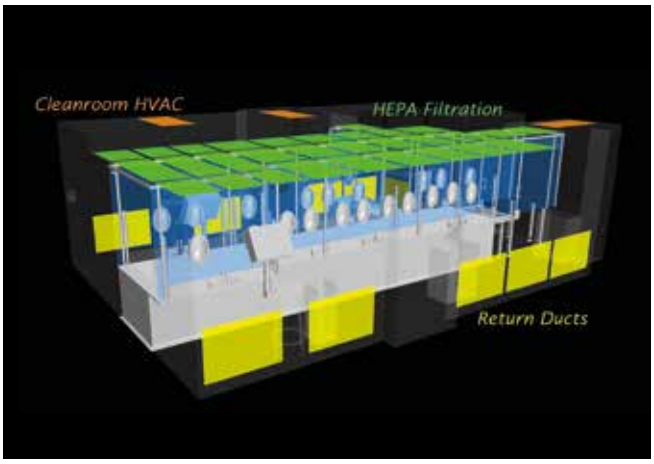


Figure 4: Principal boundary conditions.

aerodynamic deflector visible on figure 6 (b) was tested in simulation and provoked the shift of the air draft towards the machine floor. It caused the streamlines in the vicinity of the arm to reach the underside of the conveyor, keeping the potentially contaminated particles far from the vials. A similar defector was used at the level of the needles holder. Once designed by Laporte and outsourced for machining, these deflectors were tested in situ with smoke and turned out to perform very well as predicted by the CFD analysis.

Impinging flow

A third undesired situation addressed by CFD simulations is the one caused by impinging flow on nonsterile surfaces: the accumulation table and the conveyor discs. In both cases, the parts expose a horizontal surface directly to the vertical flow, inducing stagnation points and undesirable vortices.

On the table at the beginning of the production line, opened vials accumulate and form a circular pattern near the exterior edge of the table. This table is designed with a central hole, allowing for a proportion of the impinging flow to evacuate without touching the vials. Nevertheless, some streamlines evacuate through the exterior edge, passing through a series of vials as can be seen on figure 7. Many fixes to decrease head losses for the flow through the central hole have been tested in simulation with mixed success. The attention was then focused on determining the actual risk of contamination for the evacuation through the exterior edge, and a particular simulation of the flow around the vials was performed. This detailed simulation, with actual vials modeled, used the global simulation fields to determine boundary conditions. It showed that in steady-state, the entire flow in contact with the table would evacuate through the vials' shoulders (see figure 8), thus limiting the contamination risks. Laporte also proposed a specific cleaning procedure for the accumulation table.

As for the nonsterile conveyor discs, they would induce a stagnation point surrounded by vortices that would eventually transport particles over the vials path. Thus, their initial design as solid discs was questioned and Laporte ultimately remanufactured the discs and added holes, allowing for a much better

Creaform provides, amongst other services, consultation in numerical simulations and uses Simcenter STAR-CCM+ in its software arsenal as it allows them to quickly treat about any geometry, including raw scans. Our experts can work around with the scans and any other available data to numerically reconstruct the geometry and then perform the CFD simulations, cutting down costs and intermediaries.

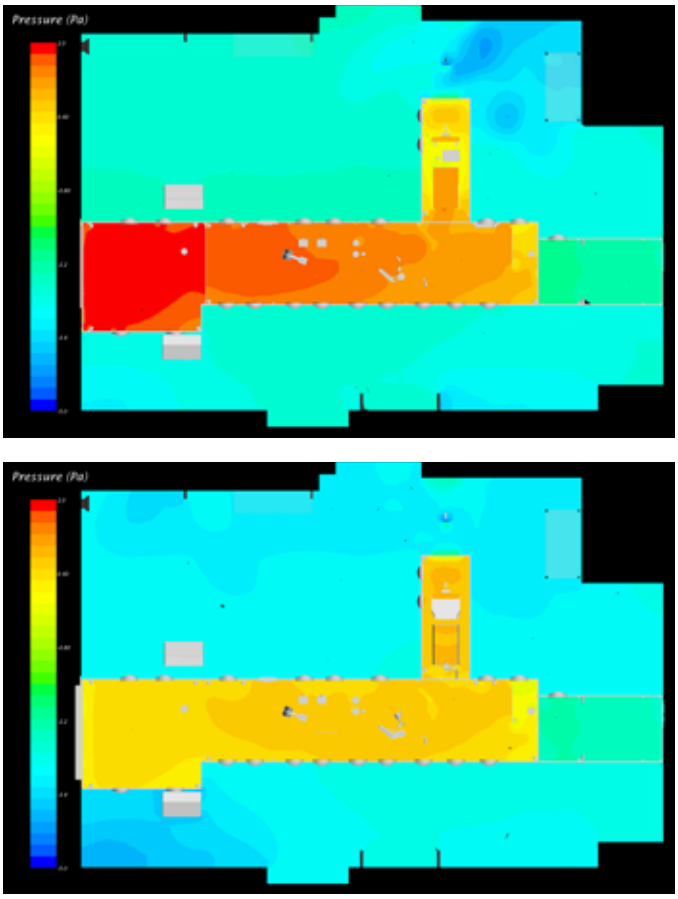


Figure 5: Pressure distribution in horizontal plane – before (above) and after (below) design adjustments.

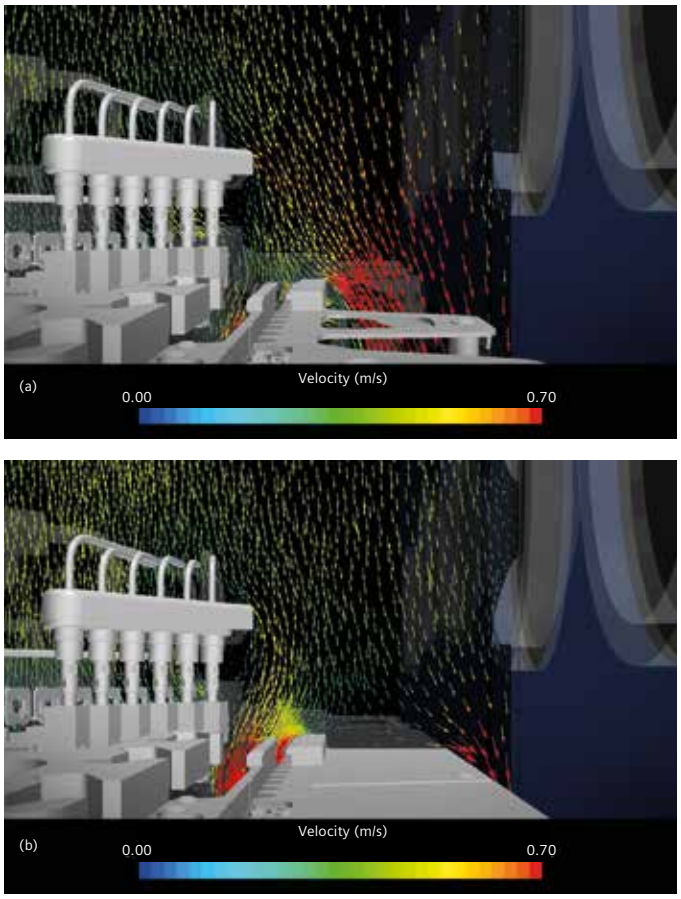


Figure 6: Velocity vectors in section plane at capping arm elbow - original design (above), modified design with aerodynamic deflectors (below).

evacuation towards the machine floor. The modification was tested with the CFD model and with smoke ejections and both methods confirmed the suppression of the issue.

Conclusion

The project was a convincing demonstration of the complementarity of the reverse engineering solutions and CFD capabilities of Creaform's Engineering Services team, equipped with Simcenter STAR-CCM+. The project was also a clear demonstration of the innovative approach of Laporte, which adopted CFD in its cleanroom commissioning in order to gain predictive insight to complement the traditional smoke tests. The CFD results presented here are currently used in combination with the smoke test videos to demonstrate the effectiveness of the aerodynamic barrier in front of regulatory agencies. So far, the feedback is very positive as CFD helps users to visualize the flow features. It is Creaform's desire to make CFD a prevalent tool for future pharmaceutical production lines. It was therefore necessary to thoroughly understand the fluid flow behavior in order to ensure proper flow path around nonsterile components of the machine. Not only was the regulatory compliance of the cleanroom at stake, but with the amazing production rate of the line (hundreds of vial fillings per minute), a contamination would represent a considerable financial loss because it would lead to wasted vaccine doses. In that context, Creaform's 3D modeling and CFD solutions came in very handy. Using basic STL files such as the ones created by 3D scanners, the engineering team numerically reproduced the cleanroom in CAD software and performed a series of CFD simulations using Simcenter STAR-CCM+.

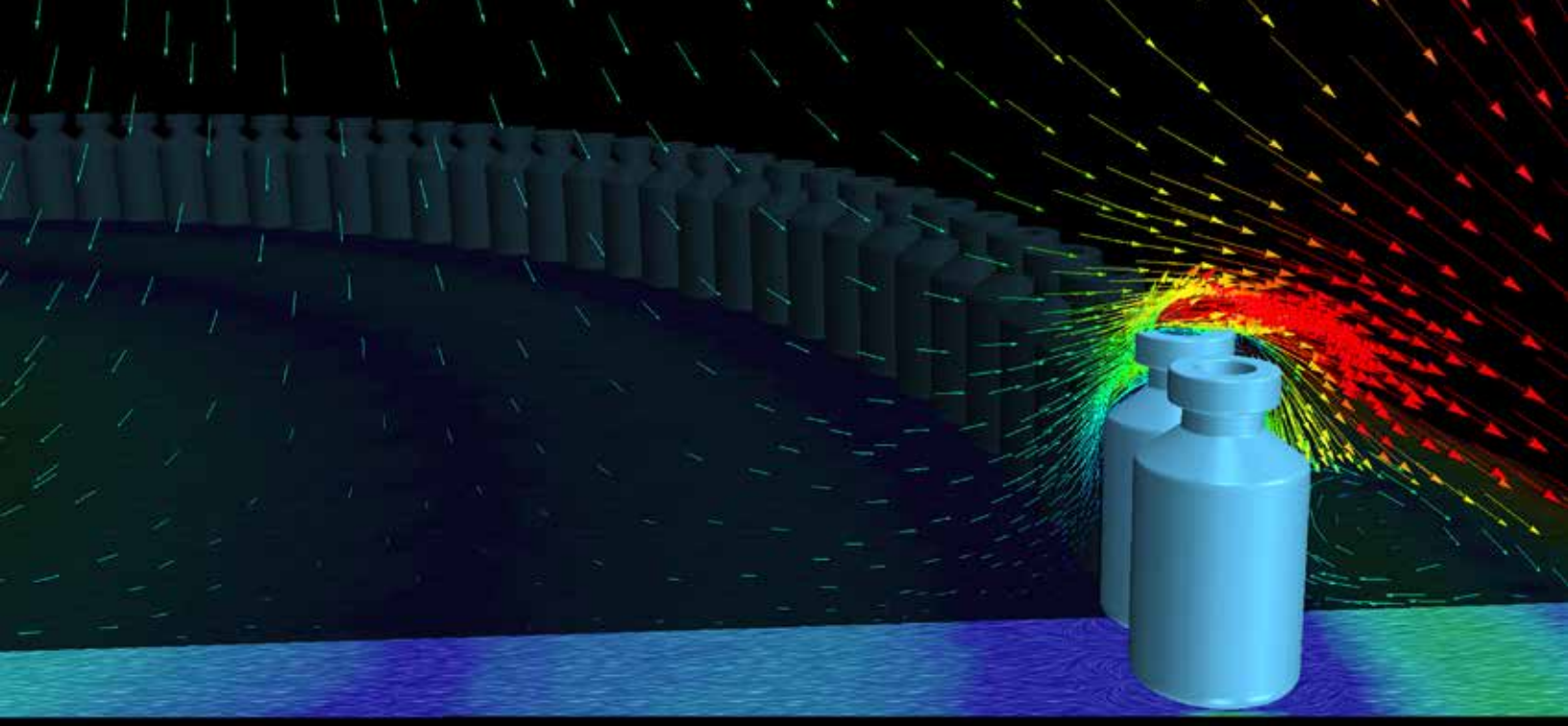


Figure 7: Impinging flow on accumulation table.

Creaform's integrated solutions of scanning, CAD reconstruction and CFD analysis gave visual and precise answers about intangible air flow questions.

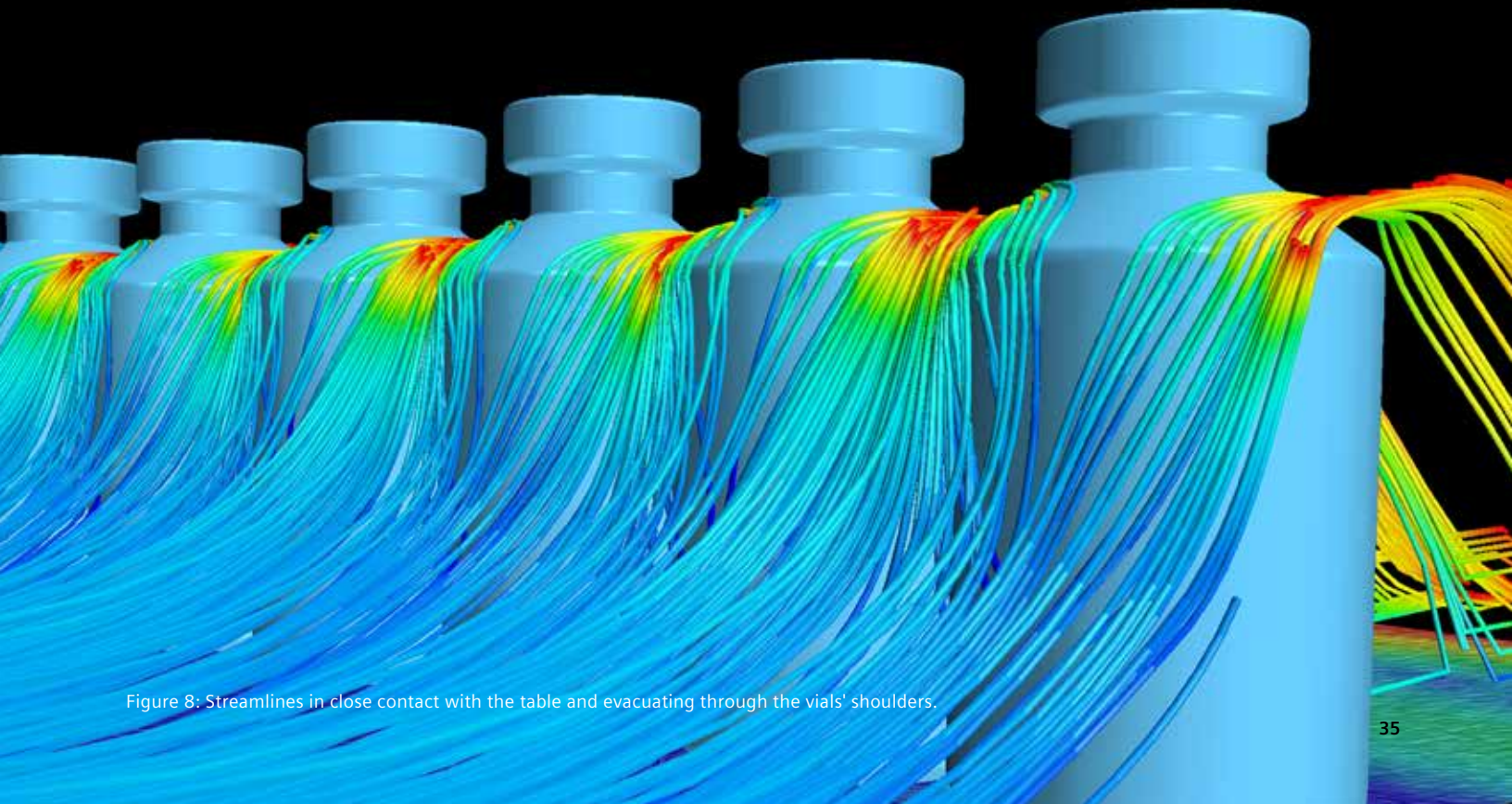


Figure 8: Streamlines in close contact with the table and evacuating through the vials' shoulders.

It's getting hot in here! Zeeco solves the mystery of a heater malfunction using Simcenter STAR-CCM+

Introduction

In engineering consulting, troubleshooting the problems faced by your customer in an efficient, timely manner is the bread and butter of the business. As such, it is highly critical to be equipped with the right tools in addition to having competent engineers tackling the problem. This article showcases one such example in which a modern numerical simulation software solution in the hands of good engineers transforms into an efficient, effective virtual troubleshooting tool. Zeeco Inc. is a provider of combustion and environmental solutions involved in the engineering design and manufacturing of burners, flares and incinerators. In addition, Zeeco also offers engineering consulting to their clients. One such customer came to Zeeco with a problematic heater that was suffering from low performance. This article highlights how Zeeco used Simcenter STAR-CCM+ software to virtually troubleshoot the heater and identify the cause of the heater's inefficient operation.

Industrial heater issues

The problematic industrial heater is shown in figure 1. The modeled system included burners on both sides at the bottom and a radiant section on top with process tubes running along the length and breadth of the heater. The convection section and stack were not included in the model. The process tubes carried processed fluids that entered the heater at the top and exited at the bottom. A combustion air distribution duct was attached to the burners to distribute the air equally to each of the burners for combustion. The walls of the heater are made of firebrick and a ceramic fiber module.

The heater had the following issues while in operation and Zeeco was tasked with finding the cause and providing solutions for these: Coking: Coking is the formation of coke on the inside of the heater tubes, reducing their heat transfer capacity. The process tubes carried hydrocarbon fluid and the heavier species in the fluid were prone to coking. During operation, it was noticed that there was coking inside the process tubes. Run length: The heater was initially designed to run for about 10 months. Due to problems with the coking, the heater only ran for three to four months after which the heater had to be shut down to clean the coking inside the tubes.

Thermal behavior: The temperature readings on the tube metal showed nonuniform temperatures and heat flux distributions at the tube surface. Visual troubleshooting of the heater and its various components is extremely difficult and impractical because there is no easy way to access the interior of the system. Zeeco decided to turn to virtual simulation to gain insight into the heater performance. Simcenter STAR-CCM+,

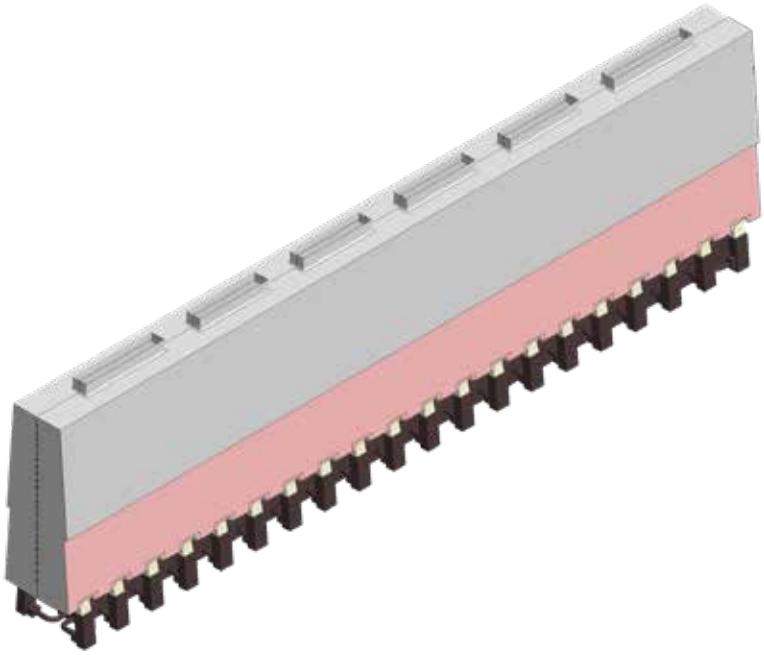


Figure 1: X-cut plane section through the gear housing showing mesh details of the model.

Siemens' multi-physics simulation software, was used as a troubleshooting tool for this purpose.

CFD setup of the heater

A CAD model of the heater geometry was prepared for analysis using Solidworks® software. The computational model included the heater radiant section with process tubes, burners and air distribution ducts. The domain was discretized in Simcenter STAR-CCM+ using trimmed hexahedral cells (figure 2) and Navier-Stokes equations were solved in these cells. Only half the heater was modeled with around 13,000 cells and symmetry condition was assumed for the other half. The computational mesh was refined sufficiently around the burners to resolve the flow field and combustion accurately. The heater was 85 feet long, around 25 feet tall and 10 feet wide and modeled in scale.

The segregated flow solver in Simcenter STAR-CCM+ is ideally suited for low-speed flows and was used here. The fuel gas mixture in the heater was refinery fuel gas, including hydrogen and hydrocarbons like methane and propane. Simcenter STAR-CCM+offers a full suite of combustion models to simulate various combustion phenomena. The multi-component species model was used to introduce the various fuel-gas components into the heater. The Eddy Break-Up (EBU) model in Simcenter STAR-CCM+ was used to model the non-premixed combustion of the species by solving the individual transport equations for mean species on the computational mesh. Ignition was not considered based on the characteristic of the heater flame and the standard EBU model was deemed sufficient to model the combustion in conjunction with the realizable k-ϵ turbulence

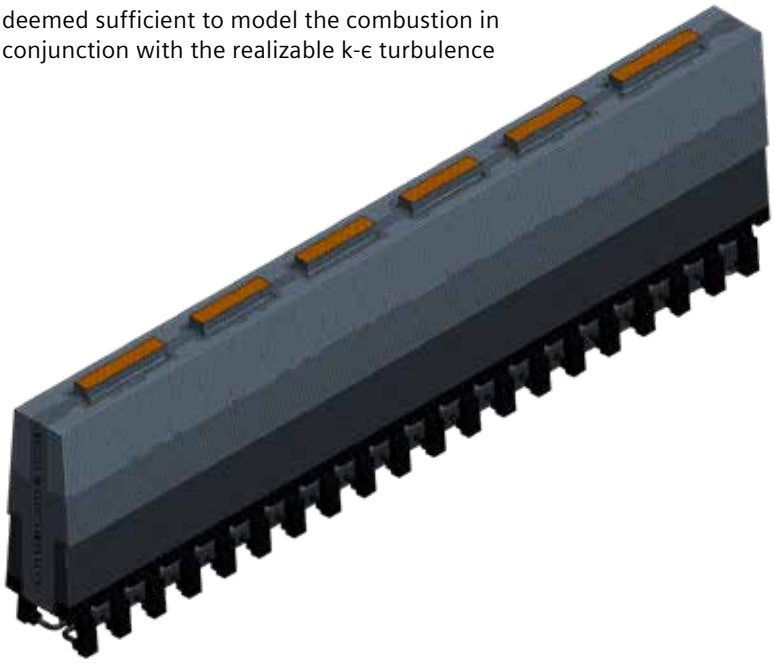


Figure 2: Initial distribution of the three different oil filling levels.

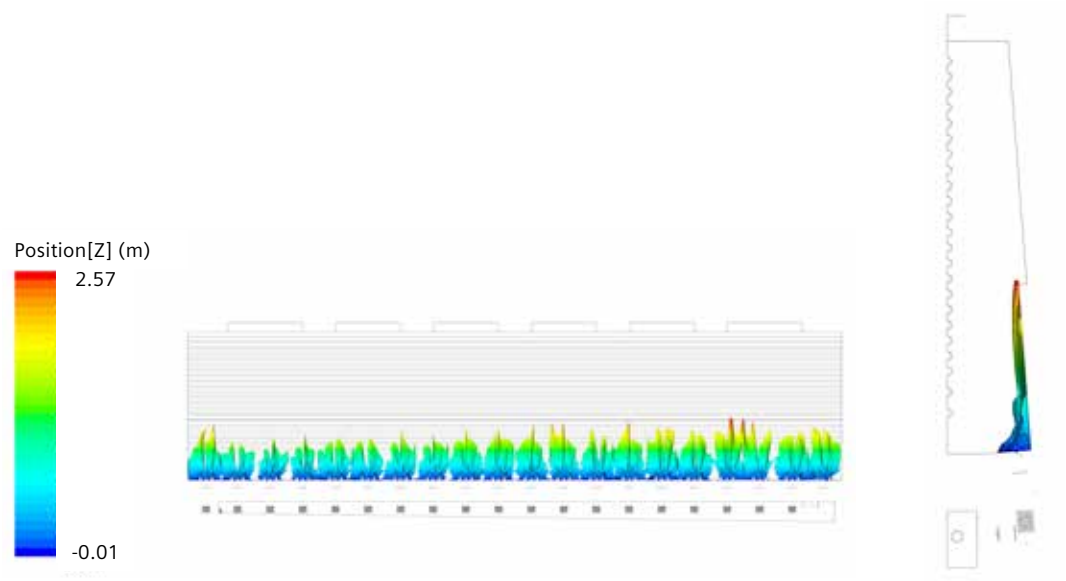


Figure 3: Oil distribution changes in time for the middle oil level.

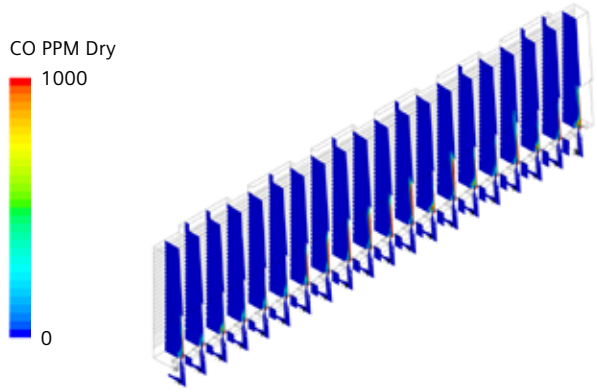
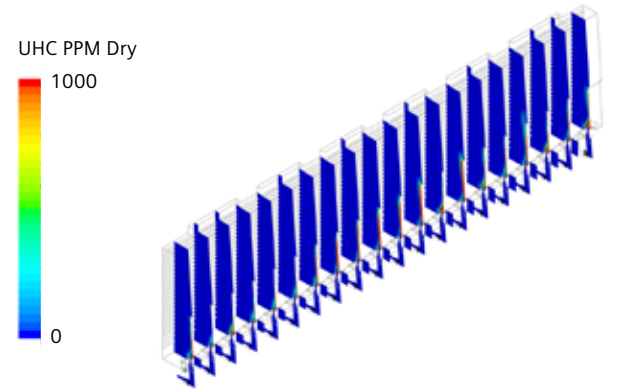


Figure 4: (a) Streamlines showing transient flow features between the intermeshing gears and (b) transient velocity flow field changes in the gearbox.

model. Radiation was accounted for by the choice of the Gray Thermal Radiation model in Simcenter STAR-CCM+.

Identification of heater issues from simulation

Figure 3 shows the predicted combustion flame profile depicted by iso-surfaces of the combustion output species. The combustion air enters the distribution ducts from right to left, leading to the flame height decreasing from right to left as the air available for combustion decreases. The burner at the far left shows anomalous behavior, with higher flame length that is caused by a special duct design at the far left end. The close proximity of the flame (front view) to the side wall was confirmed by visual observation through viewing holes in the heater. Figure 4 depicts the carbon monoxide (CO) (left) and unburnt hydrocarbon (right) concentration at the central plane of each burner, and shows the CO burns out quickly, showing that completion of combustion is not an issue. Figure 5 shows the oxygen level at the central plane of



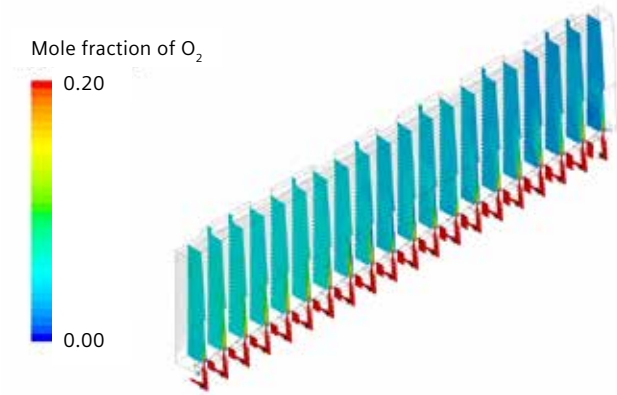


Figure 5: Pressure condition changes in time in the gearbox.

each burner. Quantitative analysis of the oxygen concentration shows that excess oxygen is around 5 percent, which is in accordance with the heater design.

The process fluid entered the heater from the top and exited at the bottom, resulting in the temperature increasing from

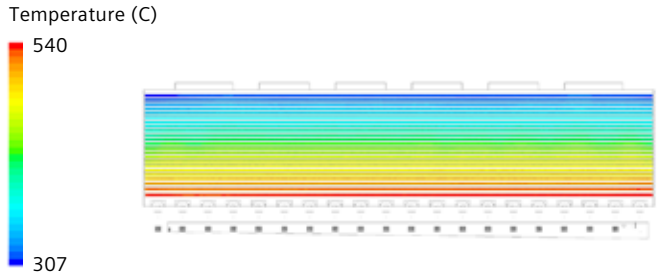


Figure 6: Volume fraction of oil between the intermeshing gears and for the three different oil filling levels at 1/3 r (additionally for filling level high at 1/2 r).

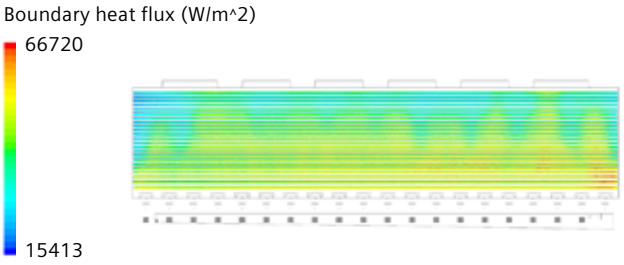


Figure 7: a) Volume fraction of oil in the gearbox and b) on gear flanks after 1/3 r and 1 r.

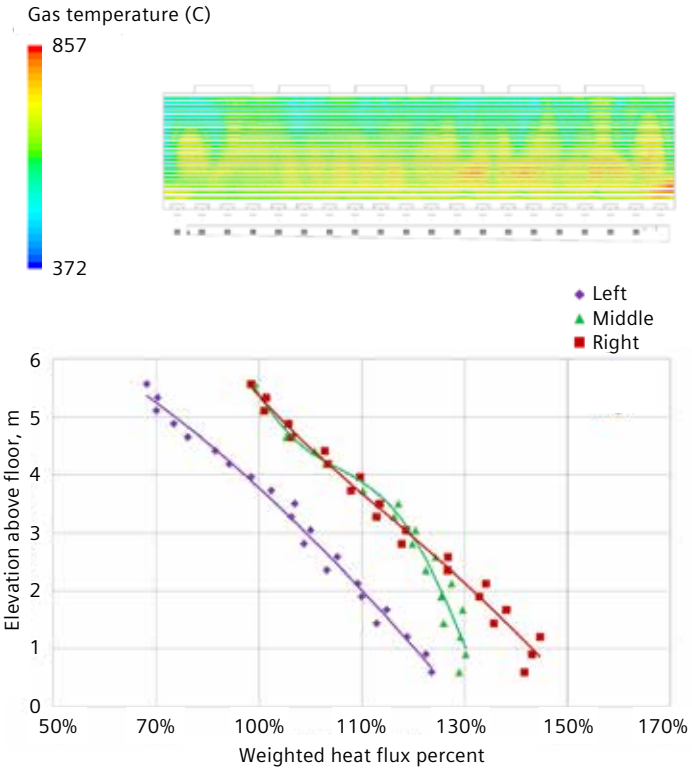


Figure 8: Temporal development of the volume fraction of oil on the flanks of gear 1 and gear 2.

top to bottom. A visual analysis of the tube metal temperature as seen in figure 6 confirms this behavior. Flue gas temperature at the tubes shows hot spots on the right side while the left side is cooler.

For any heater, a proper uniform distribution of heat flux at the tube surface is necessary for optimal operation. A nonuniform heat flux distribution results in poor heating and makes the hydrocarbons inside the heater prone to coking. Figure 7 shows the heat flux distribution on the tube surface. The left, right and middle sections of the heater are investigated to analyze the heat flux distribution. The weighted heat flux at various locations is compared for the three sections in plot 1. The weighted heat flux represents the ratio of the local heat flux to the overall average heat flux for all tube surfaces. It can be seen that the tube surface on the left is absorbing less heat than the surface on the right side.

Heater issues and recommendations

For process heaters, it is very typical to see higher heat flux at lower levels where the combustion flame enters the heater as opposed to the higher elevations inside the heater where there is a lesser heat transfer and lower heat flux. From plot 1, it is apparent that at a lower elevation, the left side of the heater has a weighted heat flux of 125 percent, while this value jumps to 145 pecent on the right side. This shows that the tube surface on the right side is absorbing 20 percent more heat than the left side, leading to coking of hydrocarbons at these higher temperatures. The heat transfer distribution on the tube surfaces is thus identified as the cause of the poor functioning of the heater. It was recommended to introduce more baffle plates and turning vanes inside the combustion air distribution duct to change the flow pattern. This will result in more uniform air distribution to all the burners, thus reducing the excessive heating of one end of the heater compared to the other.

Zeeco used Simcenter STAR-CCM+ to successfully simulate the heater operation and identify the cause of the heater malfunction. Recommendations were suggested based on the numerical simulations for improved performance. Simcenter STAR-CCM+ enabled Zeeco to solve an engineering challenge of a customer in a timely, cost-effective manner, reinforcing the capability of Simcenter STAR-CCM+ to function as a key weapon in the arsenal of any engineering consulting organization.

Picking up bad vibrations: Porter McGuffie troubleshoots a vibrating heater

The bane of most engineers is dealing with physics that have not been considered during the design process and consequently troubleshooting the problem caused by it. This phenomenon is universal across the engineering world, with operating issues in equipment cropping up in countless different ways. Some unanticipated physical behavior can easily be accommodated and fixed. Others, like those often encountered by Porter McGuffie, are much more difficult to diagnose and solve.

Porter McGuffie, Inc. (PMI), a Lawrence, Kansas-based computational mechanics and engineering measurement services company, provides engineering solutions backed by FEA and CFD analysis to a wide range of fields. One particular design problem they were asked to resolve was the piping inside a heater unit that was visibly and audibly shaking (and startling its operators). The cause of the shaking in the heater's piping system (figure 1) was unknown. The oscillatory displacement was approximately one inch in each direction under certain operating conditions. This level of vibration was considered too high for safe operation. To limit the vibrations, the unit throughput had to be lowered significantly.

To begin their analysis, PMI visited the site of the heater. They attached accelerometers to the heater's piping to get precise measurements of the vibration of the pipes. Measurements (obtained at the locations shown in figure 2) indicated the most significant vibrations were occurring at frequencies of 10 and 9 hertz (Hz), as illustrated in figure 3. Later analyses identified these frequencies as the mechanical resonant frequencies of the two separate loops in the system. Additional analysis of the vibration data revealed the envelope of the vibration amplitude had a periodicity to it. The primary period was approximately 27 seconds in length, and the secondary period was approximately 13.5 seconds in length, as illustrated in figure 4. This amplitude variation traded back and forth between the two loops in the heater, with one loop vibrating at ~10 Hz and then the other at ~9 Hz. This amplitude variation was nearly 180 degrees out of phase between the two loops.

Using this data, PMI was able to correlate the change in vibration levels to the flow of hydrogen in the two-phase distillate stream. To identify the cause of the change in hydrogen flow, PMI performed a CFD analysis on the heater piping system, recreating the entire flow regime in Simcenter STAR-CCM+. The setup made use of the Simcenter STAR-CCM+ Eulerian multiphase model to track the gas and liquid phase species in the pipes, as well as the S-gamma submodel to track the size of individual liquid droplets.

To enable tracking of various quantities within sections of the model, five regions were created: the inlet pipe, convection section, cross-over section, radiant section and the outlet tee. To accurately read the conditions of the heater, PMI set a

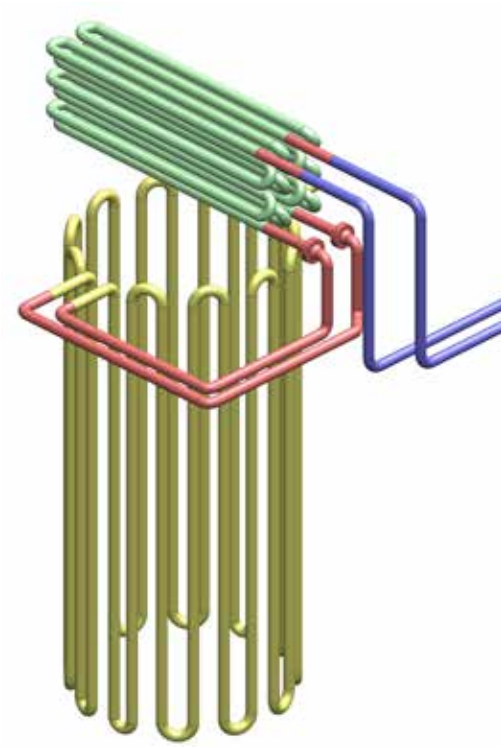


Figure 1: Geometry of piping, colored by sections.

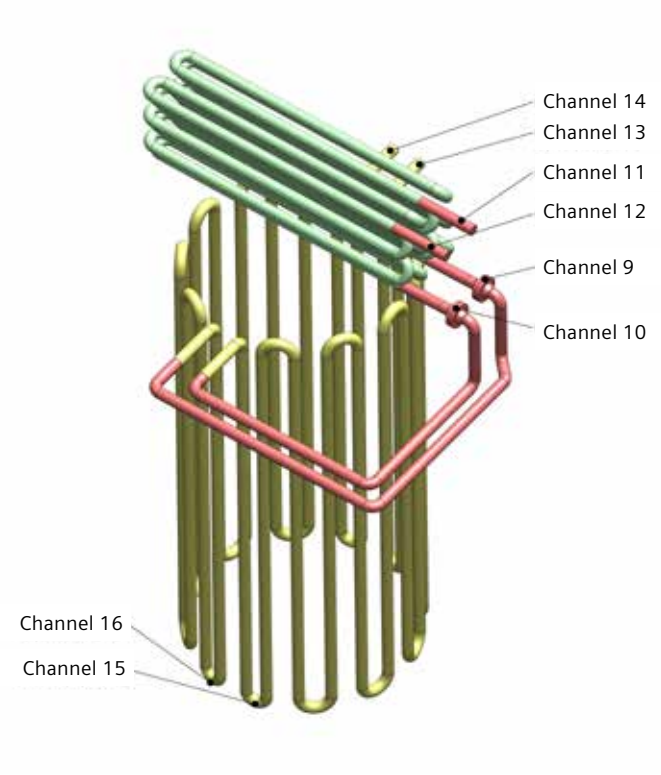


Figure 2: Locations of accelerometers on the test system.

considerable number of 3D force monitors at every elbow and pipe within the simulation as well as pressure and mass flow monitors at the entrance to each section for both liquids and gases. Flow regimes were identified within the simulation through visual inspection from still images and animations. Figure 5A shows the fast Fourier transform (FFT) of one of the pressure graphs, with the peak period oscillations of pressure indicated. Figure 5B shows the measured and simulated period of pressure pulses through the radiant and convection sections for each flow configuration. As is clearly shown, there is good agreement between the simulated and measured frequency calculations, giving credence to the time-domain pressure and force traces queried from the model.

The simulation results indicated the flow patterns in the convective region, characterized as stratified flow, did not oscillate noticeably. On the other hand, the radiative section's flow regime showed significant annular slugging (where the liquid phase flows along the wall with a gas central core) that caused highly unstable flow patterns (figure 6). The slugging pattern that formed matched the frequency of the piping vibrations. These slug patterns also correlated with the pressure pulses measured in the radiant, cross-over and convection sections. While this would be enough to provide good circumstantial evidence of the cause of the shaking, Porter McGuffie was not satisfied and investigated further, coupling the Simcenter STAR-CCM+ run with Algor (a finite element analysis code), using PMI proprietary coupling software. Applying the force load data from the CFD simulation, PMI was able to predict the displacement of the pipes (figure 7). The red highlights show the area in the heater that was having the most vibrational displacement. Figure 8 shows a comparison of the measured accelerations superimposed over the FEA-predicted accelerations, detailing obvious correlations.

Porter McGuffie was able to provide its customer with a detailed explanation of why their heater was exhibiting such high amplitude vibrations. The two-phase flow in the radiant section led to significant pressure variation in

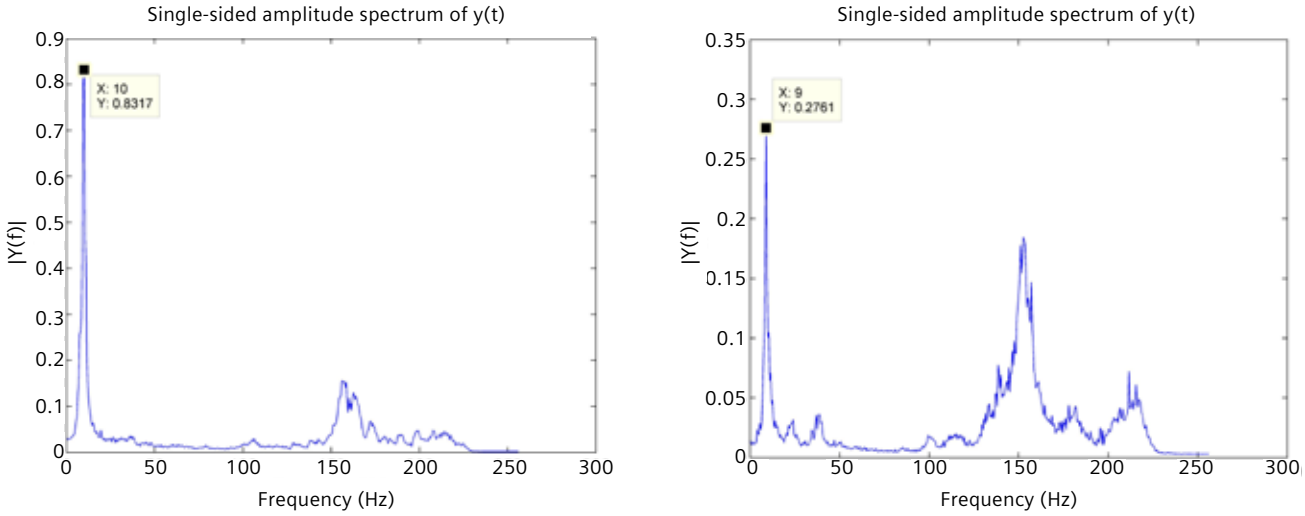


Figure 3: Vibration frequency measured at locations 9 and 10.

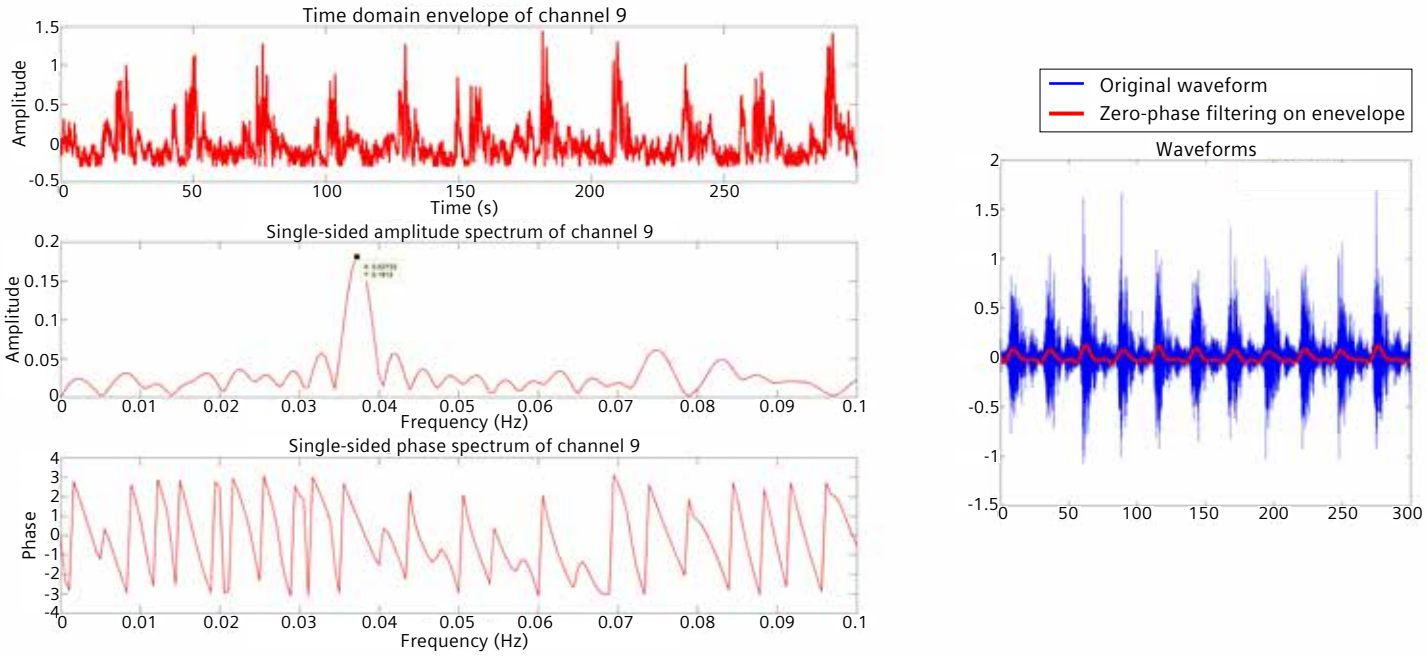


Figure 4: Analysis to periodicity of vibrational amplitudes.

the radiative section of the simulation, which caused mass flow variations in the H2 line. The pressure variation qualitatively agreed with the hydrogen flow oscillation frequency measured on site. The force magnitudes predicted in the CFD simulation and the structural vibration analysis also lined up well with the measured data. Further experimentation and simulation have shown that while the amplitude of the flow pulsations vary with overall throughput, the frequency of the piping vibration remains constant. Again, this is in good agreement with the measured data. Thus, it is clear that a resonant mode of the piping was being excited.

PMI was able to turn around the measurements and simulations within a few weeks' time using Simcenter STAR-CCM+. The use of Eulerian multiphase model with S-gamma submodel allowed the analysis of a large two-phase system that took approximately one week to run using a few million cells on 12 processor cores. The more traditional volume of fluid (VOF) model method using the correct grid density would have required more than 50 billion cells and weeks of runtime per simulation.

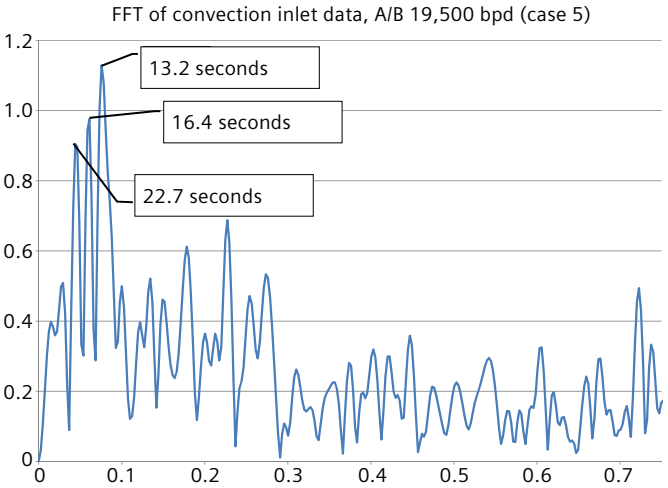


Figure 5A: FFT of pressure from time to frequency domain.

Case #	Inlet Con-figuration	Flow Con-figuration	Approximate Measured Period (s)	Primary CFD Calculated Period(s)
1	Reduced	A/B 14,500	13.3	11
2		A/B 19,500	27	23
3		C/D 14,500	13.3	14
4		C/D 19,500	27	29
5	To Exchanger Outlet	A/B 19,500	27	27
7		A/B 24,500	24.5	22
8		A/B 35,000	N/A	19

Figure 5B: Comparison of measured experimental data to CFD results.

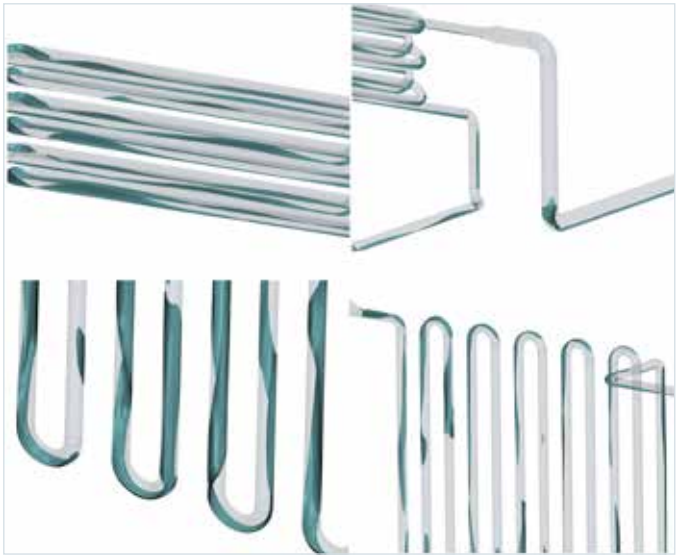


Figure 6: CFD calculated flow of liquid in the pipes, showing heavy slugging.

Mike Porter, principal engineer at PMI, stated that without simulation with Simcenter STAR-CCM+, there would have been no way to see what the fluid flow was doing within the pipes, and it would have taken many months of analysis and research to diagnose and correct the problem. All in all, Porter McGuffie was able to do the complete testing, analysis and create a recommended redesign within the span of a few weeks, not the several months' turn-around time common with more traditional methods and tools.

With PMI's suggested changes scheduled to be incorporated this October, it is nearly certain that the subject heater will be able to operate at full capacity. Porter McGuffie will then maintain its record of a 100 percent success rate for their analysis and design solutions, a claim that most engineering companies and departments within much larger corporations can only envy.

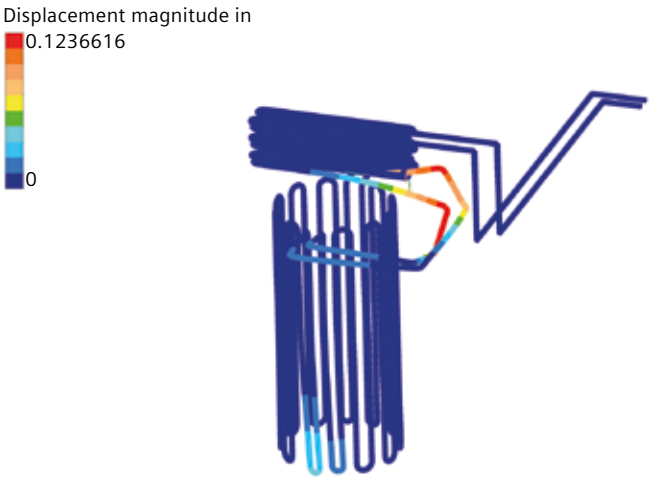


Figure 7: CFD calculated displacement of flow pipe, accurately predicting locations of heaviest vibrations.

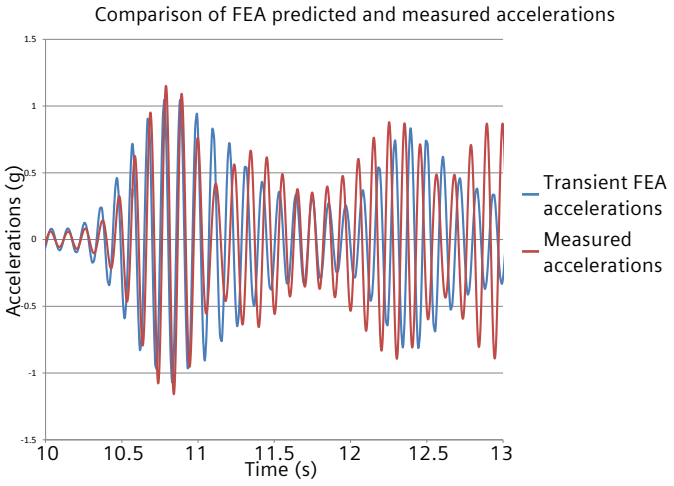


Figure 8: Comparison of FEA-predicted accelerations and measured accelerations.

A week in the life of Jane, a combustion engineer

Emission performance and drive cycle measurements for diesel engine passenger cars have created a lot of "smoke" in the media lately. The discussions highlight the importance of emission reduction and performance, and also reveal the great challenge of this work. If some of the largest car manufacturers in the world struggle to meet the emission limits, it is evident there is not an easy solution!

Emissions are by-products of a chemical process, and to understand, predict and design compliant vehicles, the underlying chemical pathways need to be well understood. The purpose of this article is to introduce you to the tools available to make the job of understanding and predicting chemistry easier and more straightforward. Let me tell you a story about Jane, a combustion chamber design engineer, and describe the daily challenges she faces.

Meet Jane!

Jane is a newly employed design engineer at CombustionCorp, a company that just started to use CFD for a major part of their development projects, the design of a combustion chamber being one of them. Jane's first assignment is to investigate and improve the design of a natural gas combustor. Using Simcenter STAR-CCM+, she is able to quickly set up the geometry and the physics, opting for the standard Eddy Break Up (EBU) combustion model. She decides that keeping it simple by just modeling one overall reaction is a good starting point as she is under a lot of pressure from her management to get the job done quickly. She obtains a flow and temperature field and verifies the results are accurate. Next, she starts her design work with Optimate+™, and is able to quickly and automatically improve the design by optimizing the fuel nozzle placement.

A few days later, a scientist from the lab tells her the combustor she is designing behaves differently for different qualities of natural gas. She wonders if she needs to consider a more complex approach and starts asking questions.

Why does the combustor behave differently for different natural gas qualities?

Different natural gas qualities contain varying amounts of larger hydrocarbons. High-quality natural gas consists mainly of methane, while low-quality natural gas includes a few percent of ethane, propane and butane. Larger hydrocarbons break much more easily than methane, and hence low-quality natural gas ignites faster.

How does the early ignition affect the overall combustion behavior?

To understand this, Jane studies the chemical effects in an isolated environment, eliminating the influence of flow fields. She finds she can use DARS to accomplish this.

DARS is a standalone tool from Siemens Digital Industries Software for analyses of chemical reactions in 0D and 1D idealized reactors. The tool can read and analyze chemical reaction schemes; for example for hydrocarbon combustion and catalytic processes in after-treatment systems.

Jane opens DARS and reads in the standard natural gas chemistry delivered with DARS.

Then she connects a few different reactors to the read mechanism module (figure 1):

- Freely propagating flame: This module calculates the laminar flame speed, which is an important property for the flame propagation and thus the combustion behavior in a combustor. The module also calculates species profiles and temperature in the flame
- Constant pressure: This module calculates ignition delay times as well as species profiles and thermodynamic properties of an auto-ignition event under homogeneous constant pressure conditions. It can also be used to calculate emission production
- Flamelet library: This module calculates the species and temperature profiles in a diffusion flame. It also calculates the extinction limit
- Equilibrium: This module calculates equilibrium species and temperature. For each module, Jane tries two different fuel qualities in DARS:
- Pure methane to simulate very high quality natural gas

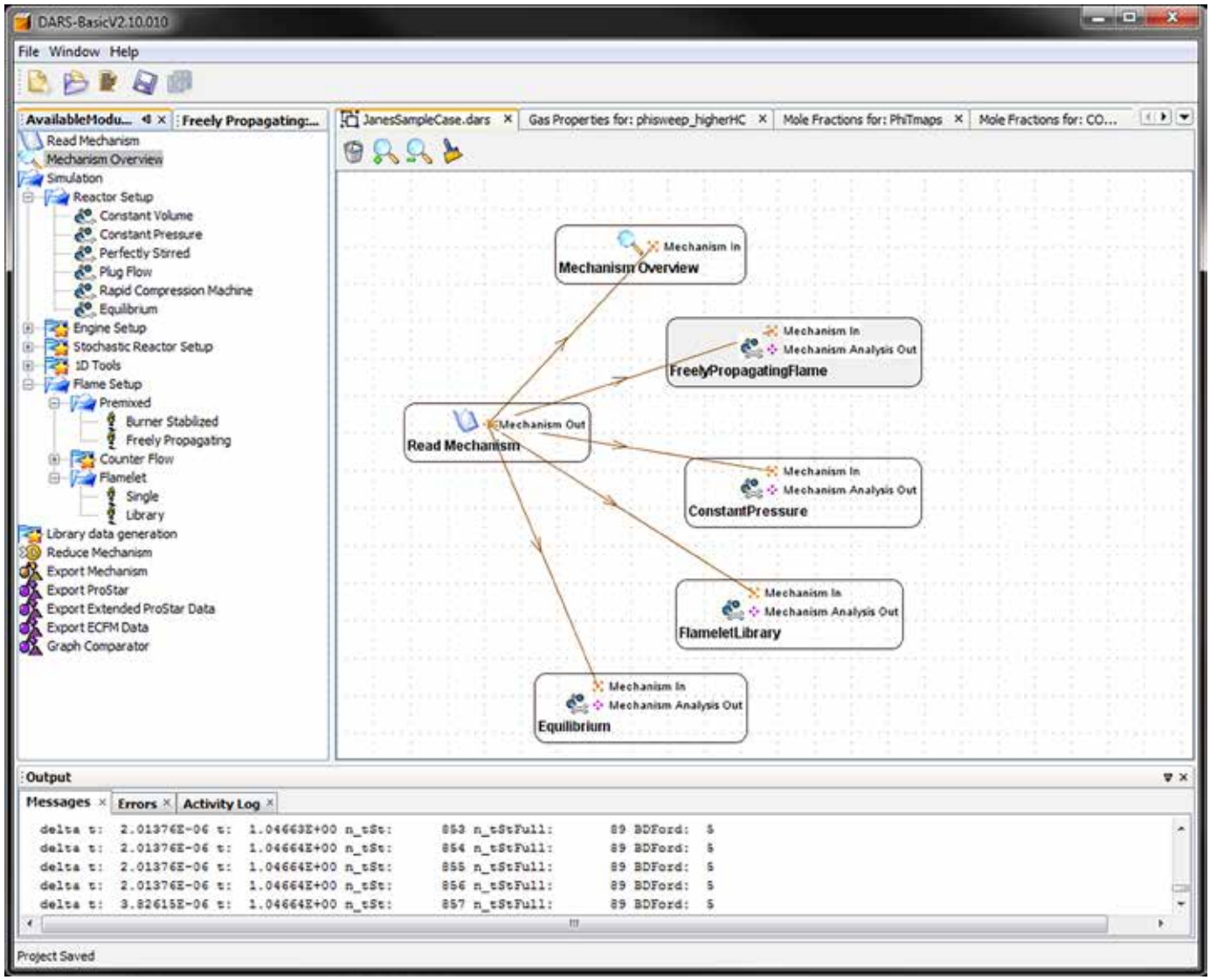


Figure 1: Case setup for chemistry analysis in DARS.

- Methane mixed with a few percent of larger hydrocarbons (C2-C4)

She first calculates the laminar flame speed for a range of equivalence ratios. The laminar flame speed is the speed of a freely propagating flame under premixed conditions. She finds the flame speed is about 1 centimeter(cm)/second(sec) faster for the low quality blend. She contemplates if this matters for her design.

What does a faster flame speed mean for the combustor?

Jane decides that this increases the risk of flashback in the combustor. She also notes that under very lean conditions,

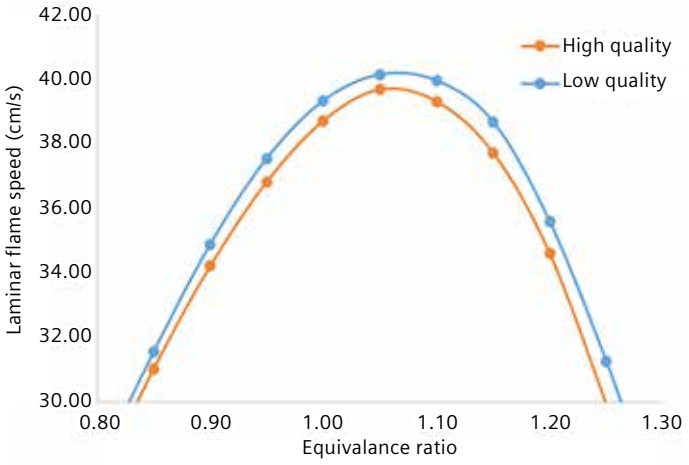


Figure 2: Laminar flame speed for high- versus low-quality natural gas.

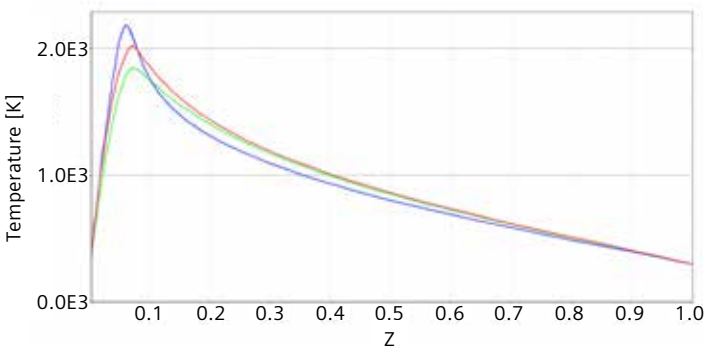


Figure 3: Flamelet temperature for low-quality natural gas for various scalar dissipation rates (green line: very low scalar dissipation rate; blue line: very low scalar dissipation rate; red line: medium scalar dissipation rate; green line: scalar dissipation rate very close to extinction).

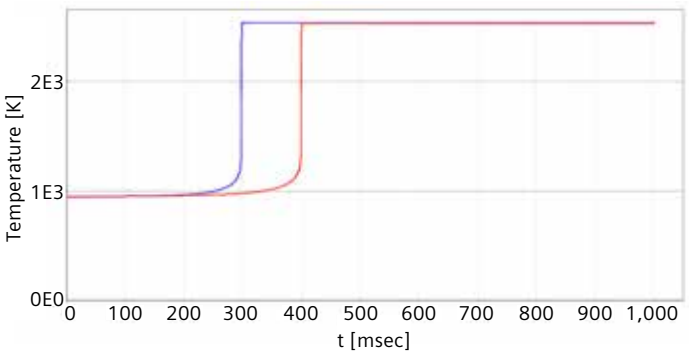


Figure 4: Ignitability for different natural gas qualities at initial temperature of 950K (red line: high quality, blue line: low quality).

the pure methane fuel speed is about 14 percent slower than the lower quality fuel, indicating the high quality natural gas is more prone to lean blow-off (figure 2).

To understand the behavior during diffusion combustion, she calculates a flamelet library for each fuel composition. A flamelet is an idealized laminar diffusion flame, and a flamelet library is a set of flamelets for various scalar dissipation (mixing) rates. She observes the maximum temperature in the flamelet is about 30,000 higher for the low-quality fuel under high scalar dissipation rate. This makes the high-quality natural gas flame more prone to extinction; she notes the extinction scalar dissipation rate is 41/s for the low-quality fuel, and 35/s for the high-quality fuel. The extinction scalar dissipation rate is the mixing rate at which the diffusion flame is blown out. This indicates that blowout is more common for high-quality natural gas (figure 3).

Jane calculates ignition delay times to understand the ignitability and to evaluate the tendency of preignition in the mixing zone of the combustor. She creates a parameter sweep (called multi-run in DARS) with methane as fuel, sweeping over the full range of fuel-air equivalence ratios given the inlet temperature and ambient pressure. After a few seconds, the calculations are finished, and she can watch the ignition of the mixture. She notes that the time-to-ignition is shortened by about 25 percent for low-quality natural gas, which gives an increased risk for preignition in the mixing zone (figure 4). From the equilibrium calculations, she observes the adiabatic flame temperature for low-quality natural gas is about 5,000 higher than for high quality natural gas. Seeing the effect on the combustion behavior with only a very slight change in fuel composition, Jane understands she needs to continue the studies in the CFD simulations to quantify the effect on the combustor behavior. She now needs to figure out several issues.

How do I account for different fuel blends in my CFD calculations?

Jane figures out that she can do this by using the flamelet generated manifold (FGM) model in Simcenter STAR-CCM+, which includes the full detailed finite rate chemistry without compromising the speed of execution. The effect of different fuel blends is accounted for by creating one FGM library for each fuel blend. The FGM library is generated from detailed chemistry.

How do I get an FGM library for my combustor conditions for Simcenter STAR-CCM+?

Jane finds out that she can use DARS for this as well. She opens her DARS project and drags an FGM library generation module to the workbench, sets up the calculations and runs the library generation. She creates a set of FGM libraries for varying natural gas mixtures and uses them in her CFD calculations, adding different fuel qualities to her Optimate+ optimizations. She finds a design that is also suitable for low-quality natural gas and delivers it to the lab engineers for testing. After this update, her colleagues are interested in the varying behavior and want to understand why this happens.

How can I understand the effect of varying fuel mixtures?

To do this, she reruns the homogeneous constant pressure reactor case with low-quality natural gas and methane only, and checks the species sensitivity analysis. The results for pure methane combustion are shown in figure 5.

As expected, methane and oxygen are the dominant species for the combustion process. Then she plots the same sensitivity analysis for the low-quality natural gas, as shown in figure 6.

Propane constitutes only 1.5 percent of the fuel blend, but still affects the combustion almost as much as methane. Butane, which constitutes only 0.3 percent of the mixture, also has a significant effect on the combustion. This shows the larger hydrocarbons have a large impact. To understand the reactions behind this behavior, she checks their sensitivities. She notices that propane and butane dissociation are two important processes, in addition to the oxidation reactions (figure 7).

Using the sensitivity analyses, plots on ignition delay times and the CFD simulations, Jane is now armed with all the material she needs to explain to her colleagues what happens during this process. A while later, the lab engineer returns and asks her about emissions. For some load points, the CO emissions are unacceptably high. Is she ready for her next challenge?

How to improve emission performance?

To better understand the CO emissions, Jane starts up DARS and runs a set of homogeneous constant pressure reactors under constant temperature, creating an emission map (figure 8).

In this map, she can see the CO production for different fuel-air equivalence ratios and different temperatures. Comparing to the mixture fraction and temperature flow field in CFD, she finds her combustor entering the CO yield area in some fuel rich zones close to the fuel outlet for the load range specified by her colleague. She needs to improve the mixing in these zones, and thus sets a constraint on the maximum equivalence ratio in these regions for the next optimization loop. She manages to decrease the CO with some efficiency penalty, and can study the trade-off between CO emission and efficiency. To further understand the CO yield, she adds CO to the postprocessing species in her FGM library generation, and regenerates the FGM libraries. Now she can directly study the CO yield in her CFD simulation (figure 9).

Finally, to fully understand the effects of detailed chemistry, she picks one of the cases and applies complex chemistry in Simcenter STAR-CCM+ to perform a full CFD simulation with the chemical mechanism used in DARS. This serves as a good benchmark against the other combustion models. She convinces her manager that although these simulations take longer to complete, they will provide much better accuracy. After all, the company doesn't want to be pulled over for noncompliance. Longer computational time might just be a small price to pay.

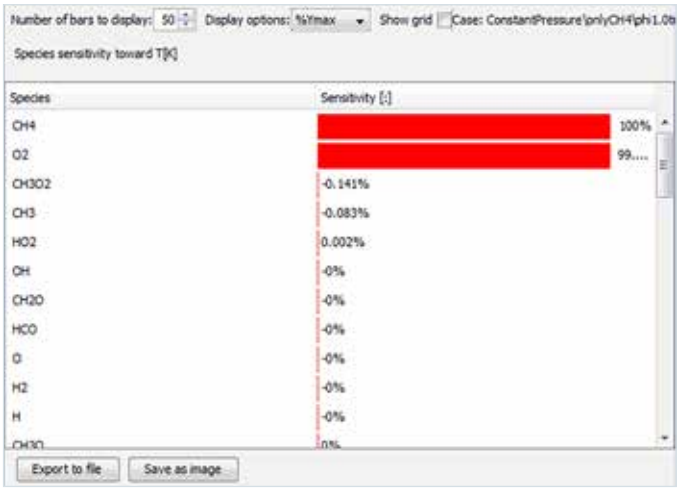


Figure 5: Species sensitivities for high-quality natural gas combustion.

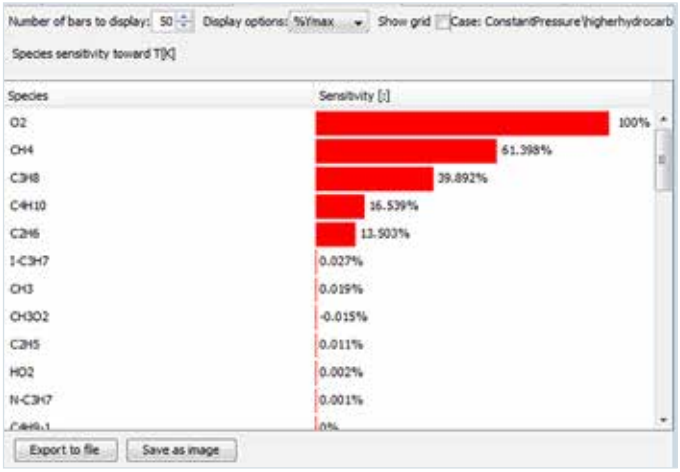


Figure 6: Species sensitivities for low-quality natural gas combustion.

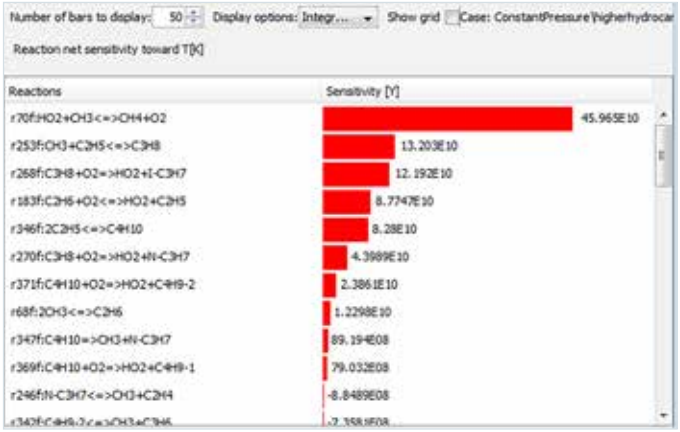


Figure 7: Reaction sensitivities for low-quality natural gas combustion.

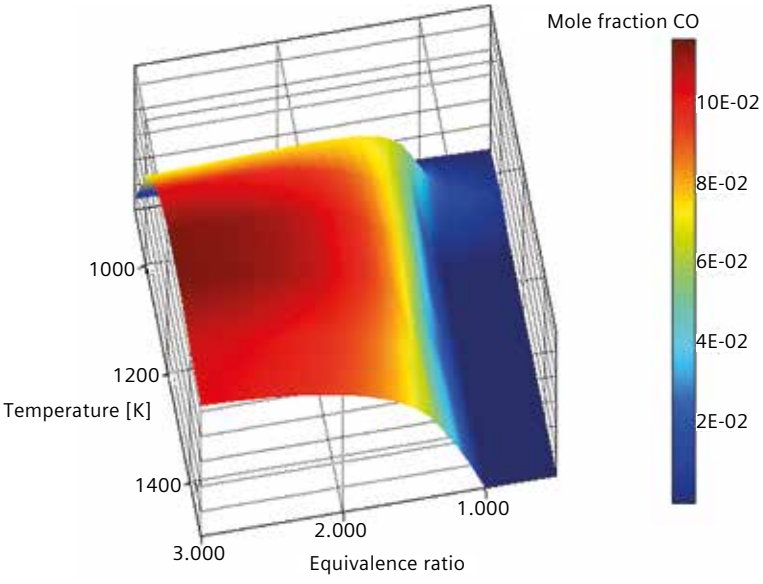


Figure 8: CO emissions as a function of temperature and equivalence ratio.

Additional information about DARS
In addition to performing the complex chemistry calculations described in this article, DARS can be used to:

- Generate combustion and emission libraries for in-cylinder combustion:
  - ECFM-3Z TKI
  - ECFM-CLEH TKI + Equilibrium
  - PVM-MF
  - Soot
- Calculate laminar flame thickness
- Calculate surface and gas phase chemistry in catalysts (DOC, TWC, DPF, etc.)
- Reduce mechanisms
- Calculate in-cylinder combustion using stochastic reactor models

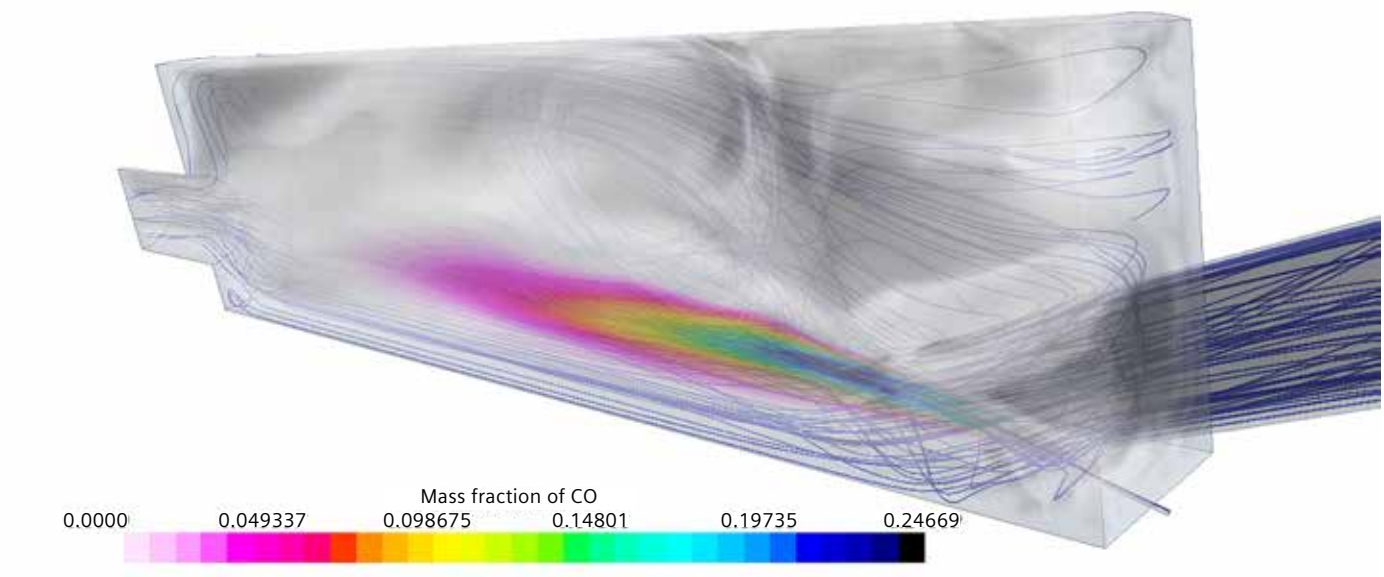


Figure 9: CO mass fraction field in glass furnace simulation using the FGM combustion model.

From gob to bottle: Bottero simulates the complete glass forming process

Introduction

Glass container production is generally not an easy process to operate and companies often need to invest a significant amount of time and money to ensure they deliver products with appropriate quality. Glass is indeed a material that exhibits extremely complex behavior, which is often difficult to predict during manufacturing. Until now, the tuning of the production parameters has been completely bound to the operator's experience.

To overcome this sticky situation, Bottero, a process-oriented company operating worldwide in the glass machinery field, has developed a simulation-based methodology in cooperation with university laboratories and production experts. The aim of this work is to provide glass plants with the necessary support for manufacturing tools to ultimately achieve a drastic reduction in the time required for starting up a process.

Computer simulations are not only useful to gain a better insight and assist in designing optimal bottle shapes, they also offer a good alternative to time-consuming and expensive trial-and-error procedures commonly encountered by factories. Representative numerical simulations can help minimize unwanted variations in wall thickness of containers and reduce their weight while maintaining their strength. Simulations also are extremely valuable in optimizing cooling conditions and increasing the production speed. All this has the potential to significantly decrease the cost of the glass manufacturing process.

The glass container forming process

During the process, the container is first formed into an intermediate shape, called the parison, and then blown into its final shape. Depending on the different ways of forming the parison, two glass processes exist: the blow-and-blow, in which the parison is formed using compressed air, or the press- and -blow, in which the parison is mechanically formed with the use of a plunger. Here, the press-and-blow process has been studied and simulated.

When the molten glass leaves the furnace, its temperature is over 1,400 Celsius (°C) as it goes through the foreheart and then the feeder and is cut into uniform gobs of glass by a shearing and distribution system. After this, each gob is sent to an individual section forming machine where the temperature drops below 1,200°C, and the gobs are forced to take the mold shape. The forming machine consists of two sets of molds called the blank and blow molds.

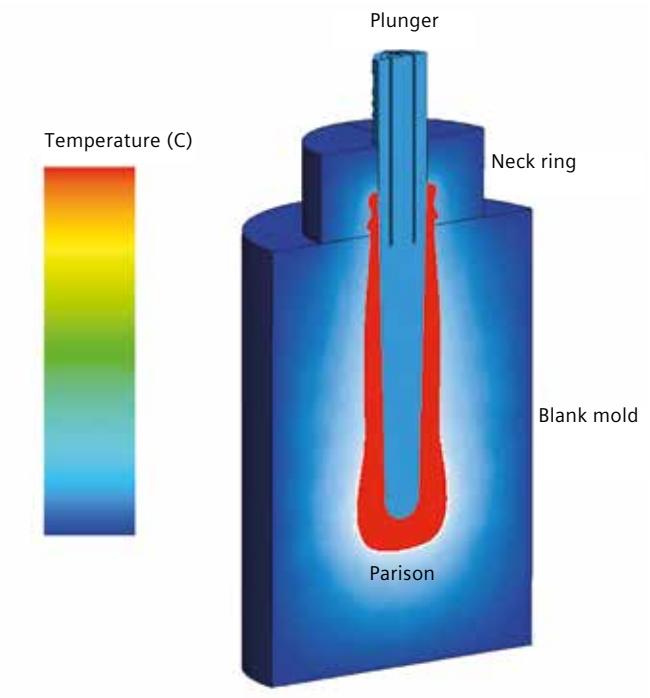


Figure 1: Three dimensional temperature distribution of the parison as it is created in the blank mold.

First, in the blank mold, the gob drops from above and is pressed into the mold shape, forming a thick-walled preform or parison. This parison is then removed by a robotic arm from the blank mold, turned upside down and transferred to the second (blow) mold. At this moment, the preform starts to stretch towards the bottom of the mold due to gravity. Finally, pressurized air is injected and a vacuum is created to inflate the parison into the final bottle shape. The container is then transferred to an annealing oven where reheating removes the stress produced during forming. After this, the container is cooled under controlled conditions and the process is complete.

The need for simulations for glass forming

The glass forming process involves high temperatures, and it is extremely sensitive to changes in machine timing, glass composition and environmental conditions. As it is nearly impossible to physically visualize what happens inside the molds during the different phases, numerical simulation is the only tool available to help better understand the details of the physics as they occur during the process. In this work, the results of the simulation are validated experimentally by comparing infrared surface temperature measurements of both glass and equipment and inspecting the final container, the glass distribution (wall thickness) and the presence of possible defects. In building the simulation methodology, close attention was paid to ensure the most realistic model possible was used. This means that approximations in the simulations were limited and the glass forming process was modeled as a tightly coupled thermofluid-dynamic process. In the process, the hot glass yields heat to the molds through conduction and radiation, and the glass is only partially emitting/absorbing the infrared light. Additionally, a heat exchange also occurs between glass and environment through convection and radiation. These heat exchange interfaces are geometrically complex and drastically change in time during the shaping of the bottle.

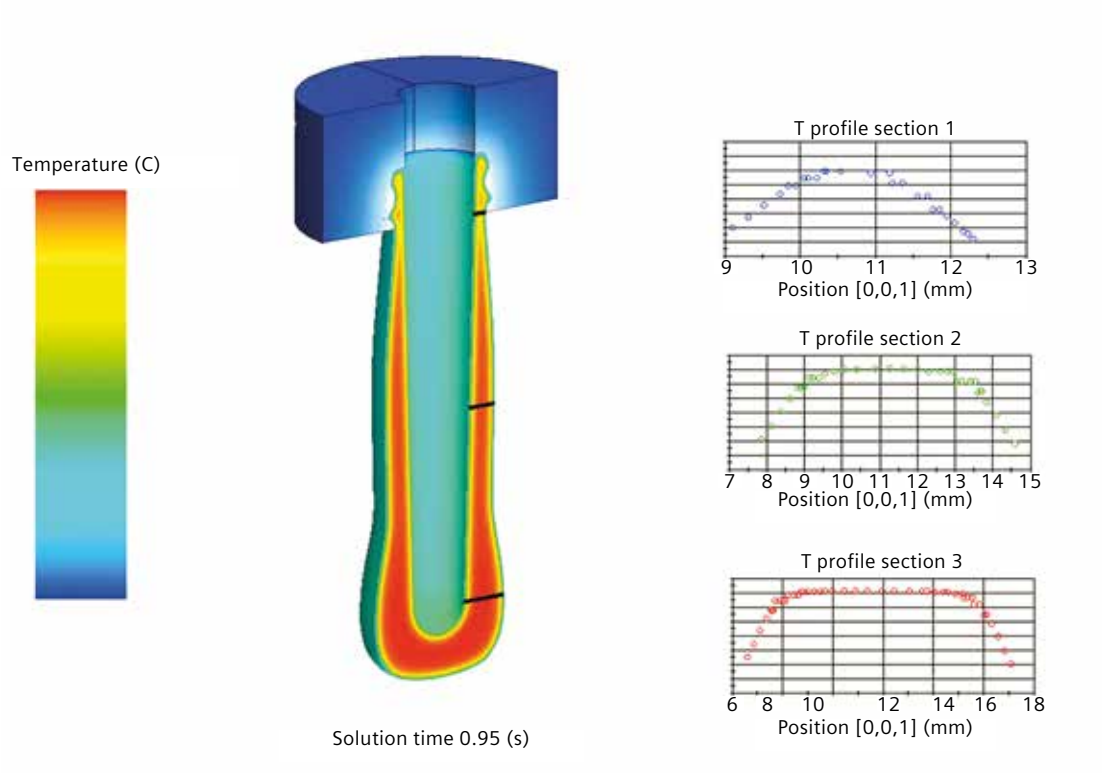


Figure 2: Detailed 3D temperature model of the parison showing realistic vertical temperature trends.

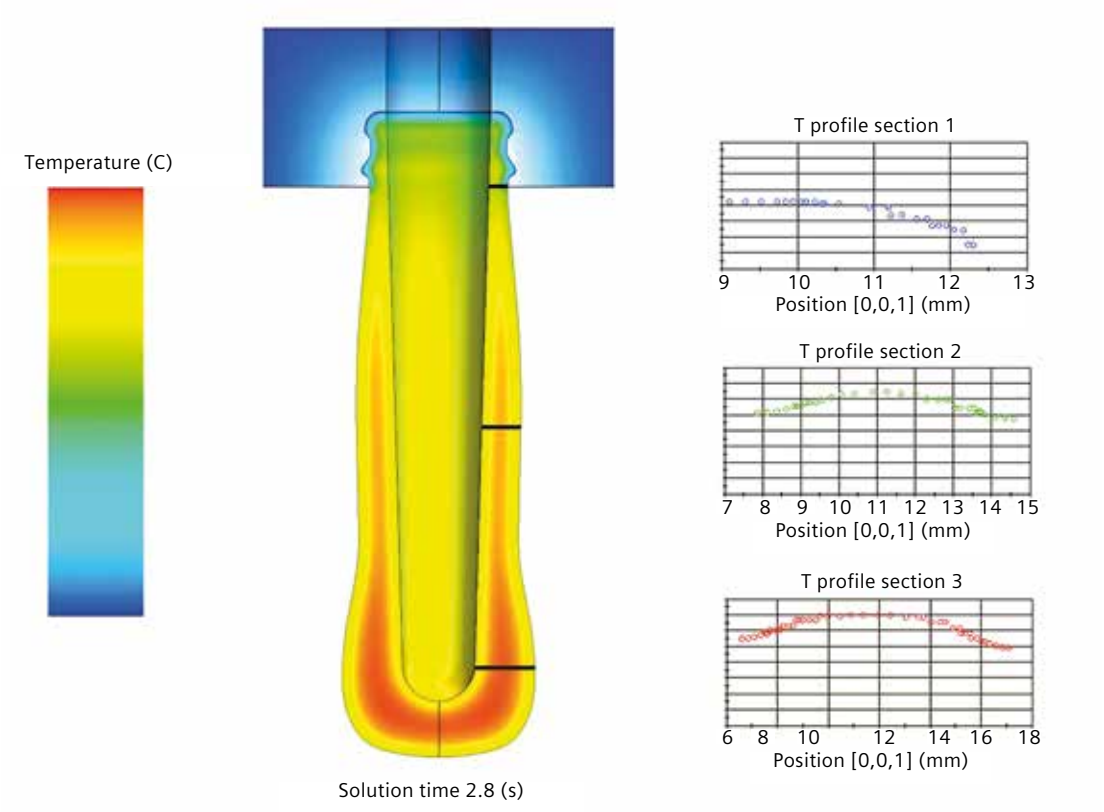


Figure 3: Parison temperature during reheating showing temperature redistribution.

Figure 4: Experimental tests were conducted on the glass and confirmed a good correlation with simulations

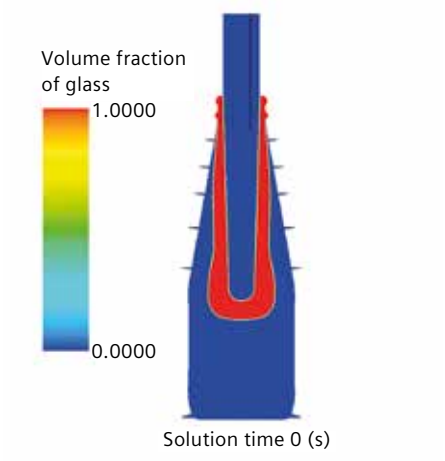


Figure 5: Volume fraction of glass in the dynamic model of the parison for simulating shape changes.

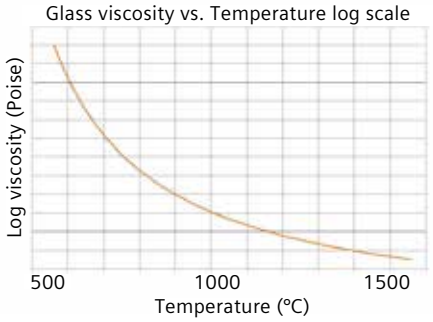


Figure 6: Variation of glass viscosity with temperature during the glass forming process.

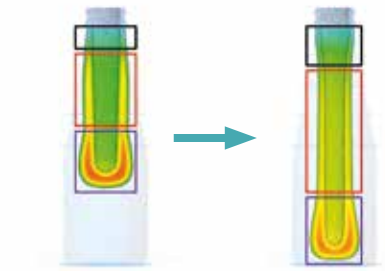


Figure 7: Simulation with Simcenter STAR-CCM+ showing the shape change of the parison in the blow mold.

The modeling methodology

Simcenter STAR-CCM+ has made it possible to simulate the complete physical system of this production cycle, starting from a hot glass gob all the way up to the creation of the finished bottle. A super-computing facility located in Cuneo, Italy (with 25 servers available that operate concurrently on high-performance computing clusters with over 450 cores) facilitated CFD simulations with a very fine volume mesh, resulting in a large number of elements and ensuring a great space resolution to accurately capture the forming process.

The first step in developing the process was to perform unsteady simulations to obtain the three dimensional temperature distribution of the parison created by pressing the glass gob into the blank mold (figure 1). The numerical model was initialized using the experimental conditions (such as temperature profiles), included all the details of the equipment and solved for both discrete ordinate model (DOM) radiation and conduction. The contact heat transfer coefficient at the interface between glass and cast iron is not only a function of temperature, it also depends on many other parameters (for example time, pressure, mold roughness, presence of lubricants, etc.), thus it cannot be considered to be an ideal coefficient. For the simulations, the heat transfer coefficient used was determined by experiment.

The transient simulation led to a detailed 3D temperature model of the parison, and showed realistic temperature trends as expected: the glass was hotter where the parison wall was thicker. This typical vertical temperature trend is required to form a good final product and can be very tricky to control in experiments. As expected, because the glass viscosity depends on its temperature, the cold neck zone behaved as solid glass while the hot bottom of the parison was still soft and easy to work with. A similar approach was used to simulate the reheating of the parison, when the mold opens and the parison temperature redistributes along the thickness for about two seconds (figure 3).

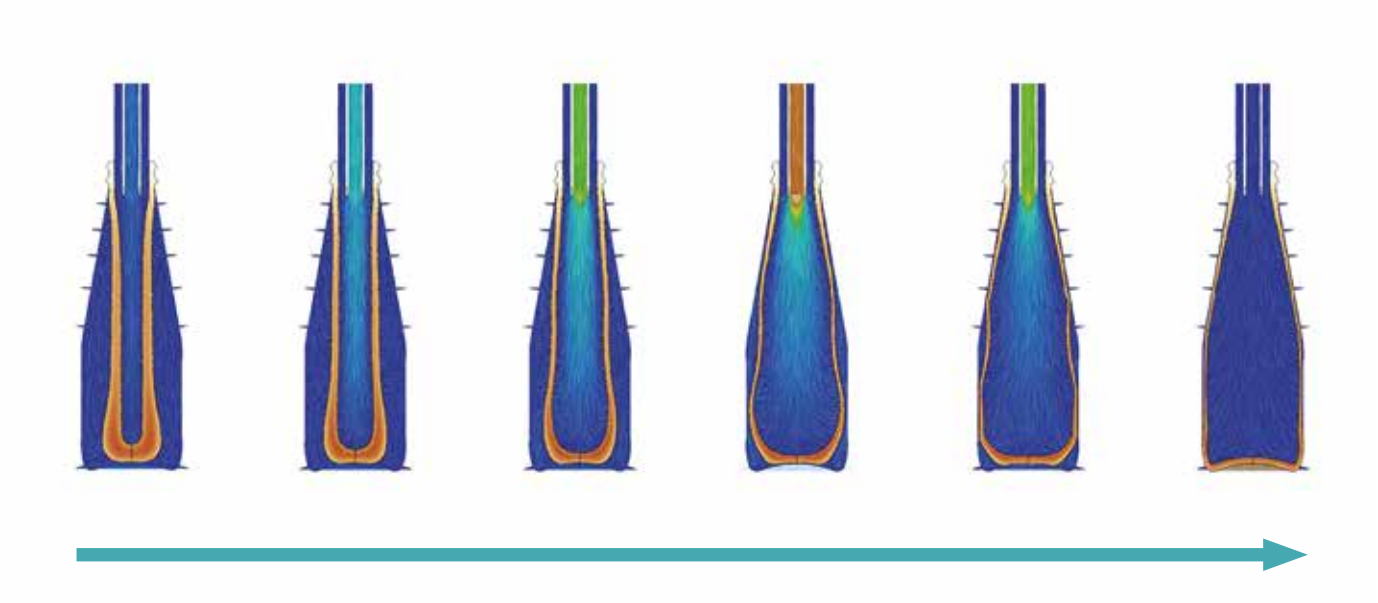


Figure 8: Complete simulation with Simcenter STAR-CCM+ for the glass forming process, starting from the initial glass gob to the final shape.

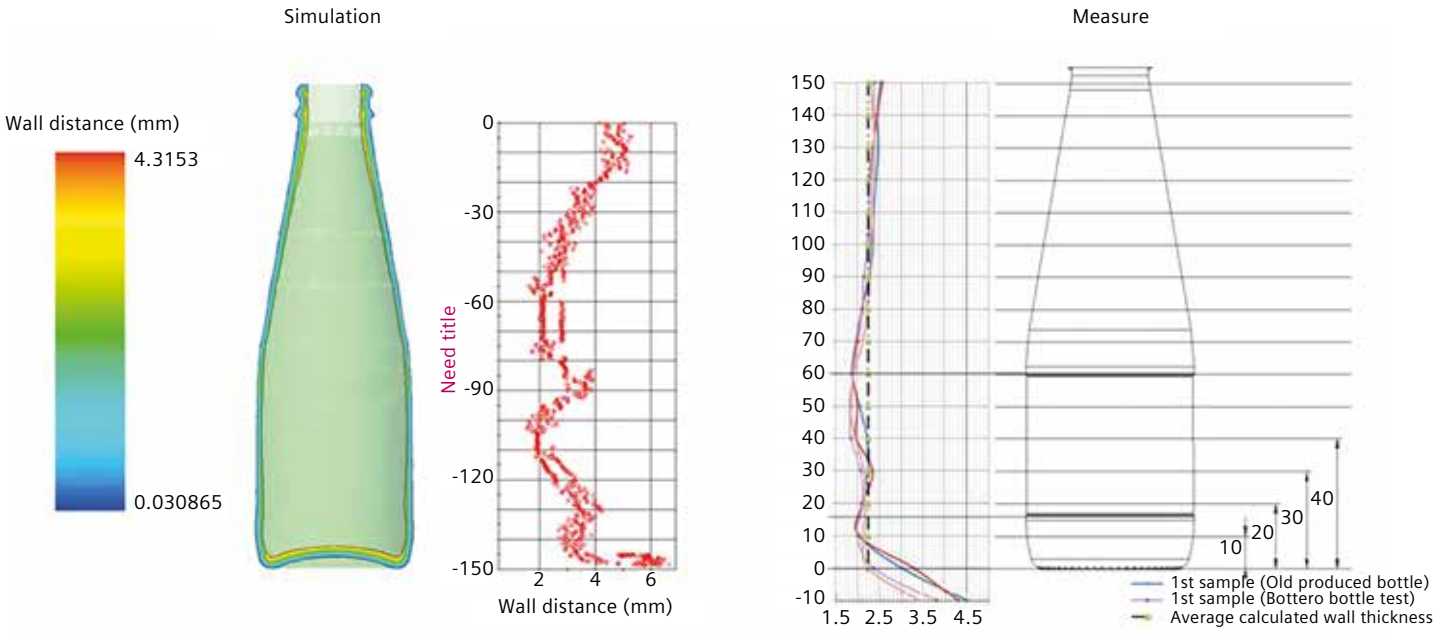


Figure 9: Validation of numerical simulations with Simcenter STAR-CCM+ showing good comparison when comparing wall thickness to real bottles.

Simulations with Simcenter STAR-CCM+ were useful not only for calculating the complete volume temperature (surface and internal) of the parison, but also for better understanding the available thermo-infrared measurements of glass and molds as these give information only on the surface and not on the inner part of the parison. Experimental tests on the glass were conducted (figure 4) to verify the simulation results, confirming good correlation between simulation and experimental data.

Next, a dynamic model of the parison for predicting the shape changes that occur in the blow mold was built, with the simulations starting from the initial temperature distribution obtained in the previous step. This is one of the most important steps in the glass forming process as it greatly affects the final bottle shape. The Volume of Fluid (VOF) model in Simcenter STAR-CCM+ was used to model both fluids in the simulation: glass (dense and viscous) and air that surrounds the parison (figure 5).

The VOF method allowed for accurately modeling the details of the glass and air flow, separated by a well-defined interface (free-surface) and solving for its position in a time-accurate manner at every time-step. Mechanical and thermal properties of the materials were taken into account, including viscosity, density, conductivity and specific heat. Additionally, since the viscosity of glass depends on temperature, and the temperature changes with time, the heat flux and temperature distribution in the simulation were solved simultaneously with the motion of the interface.

Using the experimental measurements of the specific glass viscosity as a function of temperature (figure 6) and the temperature profile obtained in the previous step, the mechanical behavior (shape change) of the parison was successfully simulated as it developed in the blow mold. The model consisted of the inner surface of the mold that corresponds to the final bottle shape.

A pressure inflow in which the air is injected was included on the top and several pressure outflows were present on the sides for creating the vacuum in the final step of the process.

For the first 2.2 seconds in the blow mold, the parison stretches down to the bottom solely due to gravity, so no air is injected. This process, also called stretching, is crucially important to get the right thickness of the bottle wall, and it is extremely sensitive to the parison temperature as it affects the viscosity of glass.

Looking at figure 7, simulations showed that starting from the top of the parison in the neck region, the glass was cold so it resisted stretching even with a high gravity load from below present. Furthermore, it became clear the central part of the parison was most responsible for stretching while the bottom (with the lowest gravity load) did not stretch even if glass was soft.

This physical process was successfully simulated thanks to the simultaneous prediction of both the dynamic and thermal features in the Simcenter STAR-CCM+ model. This allowed for taking into account the temperature redistribution of the glass during reheating (and thus the local time-accurate viscosity change) while stretching occurred.

During the final step in the simulation of the glass forming process, air was injected from the top and a vacuum was created from the side holes to blow the shape into the final bottle, as shown in figure 8. Even though this fast motion is not trivial and presents a challenge, the solver remained stable throughout the simulations.

The simulation results were validated by comparing the wall thickness of real bottles with the values obtained by simulating the process (figure 9). The correlation was very good, confirming the numerical model is robust, especially considering it is the final result of many consecutive steps. This should come as no surprise since great care was taken to ensure the numerical model represented a realistic process, taking into account the glass (whose properties are strongly influenced by the temperature), the air, the molds and all the production equipment. The glass data has been experimentally measured in a specialized laboratory, and the experimental machine timing was also considered.

Conclusion

In this study, we presented the numerical implementation of the forming process of glass containers that was previously tested in realistic manufacturing conditions. Both the press and the blow steps of the forming process were modeled using Simcenter STAR-CCM+. A realistic nonuniform temperature distribution of the parison was calculated and the final shape of the end product was presented and analyzed.

All calculations were performed in three dimensions, which allowed for studying parisons that are not rotationally symmetric, enabling one to assess how a certain imperfection in the initial parison develops over time. The current model is valid for viscous fluids, but it could be modified to, for instance, visco-elastic fluids.

The numerical simulations presented here are extremely valuable to the glass manufacturing industry as they help gain insight into the details of the physics, enable optimization of the production process and will ultimately lead to a significant reduction in manufacturing time and cost.

Simulating laser welding shortens design cycle and optimizes component design at Owens Corning

It wasn't your everyday assignment. Byron Bemis, senior research associate at Owens Corning, and his team were asked to design a new generation of manufacturing components that could not be made using existing manufacturing processes. Owens Corning is a leading global producer of residential and commercial building materials, including insulation and roofing shingles; glass-fiber reinforcements for products such as cars, boats, wind blades and smart phones; and engineered materials for composite systems. Its Science and Technology Center, where Bemis is located and much of the company's research and development (R&D) takes place, is in Granville, Ohio.

With this particular RandD project, Bemis and his crew were breaking new ground. To design and fabricate the requested parts, their initial designs called for blind keyhole welding through one sheet metal part and into another. "Developing the welding parameters to make those welds work reliably and robustly took a lot of trial-and-error," Bemis says. "To accomplish this using physical prototypes meant fabricating the individual component parts and then laser welding them up using a set of predetermined parameters to see what happens. You continue doing this until you find the right combination." Bemis adds that one of the most challenging aspects of this project was the necessity to weld close to small features or near corners or edges. If the laser is running too hot or moving too slowly, the feature or edge could melt, ruining the part.

These were small welds, varying in size from millimeter to submillimeter scale, made on very small parts that demanded high precision fabrication. Bemis says they were running narrow weld beams — in many cases 50-micron weld spots using up to a kilowatt (kWh) of laser power on an individual spot.

The materials used were alloys with high melting points, high molten metal viscosity and surface tension. This made for some interesting, nonstandard welding physics.

Complex geometries were also involved, including small features, edges and circular sections. Because deep penetration was necessary to make the part, a keyhole mode was required. Keyhole mode is a welding technique in which a concentrated heat source, such as a laser, penetrates completely through a work piece, forming a hole at the leading edge of the molten weld metal. As the heat source progresses, the molten metal fills in behind the hold to form the weldbead. All of these considerations - in particular, the blind keyhole welding - meant a lot of trial-and-error. Running hundreds of repeated physical experiments using expensive alloys

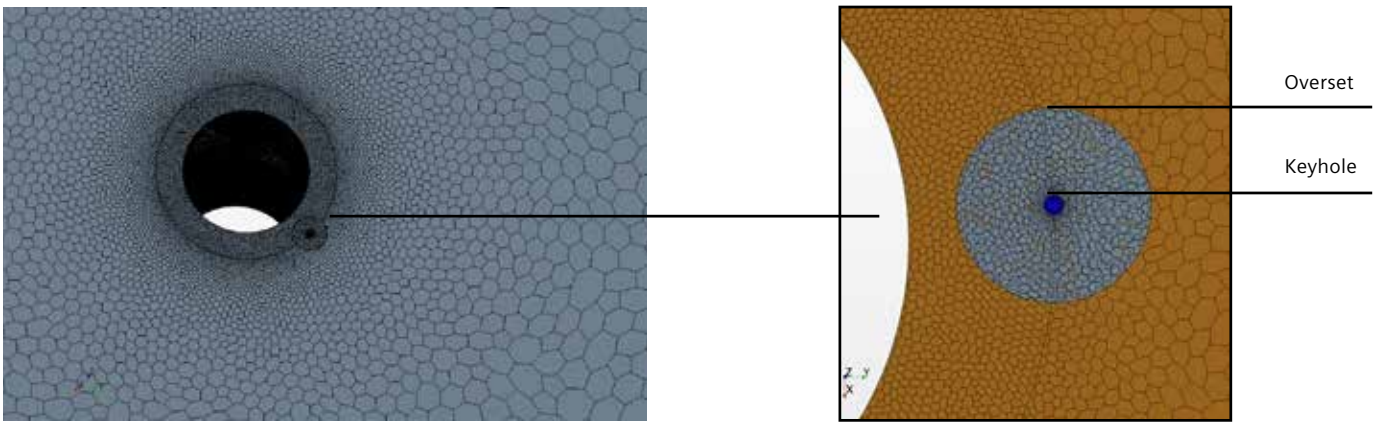


Figure 1: One of the unique features of Simcenter STAR-CCM+ that Bemis found extremely useful was overset mesh, a major advance in simulation.

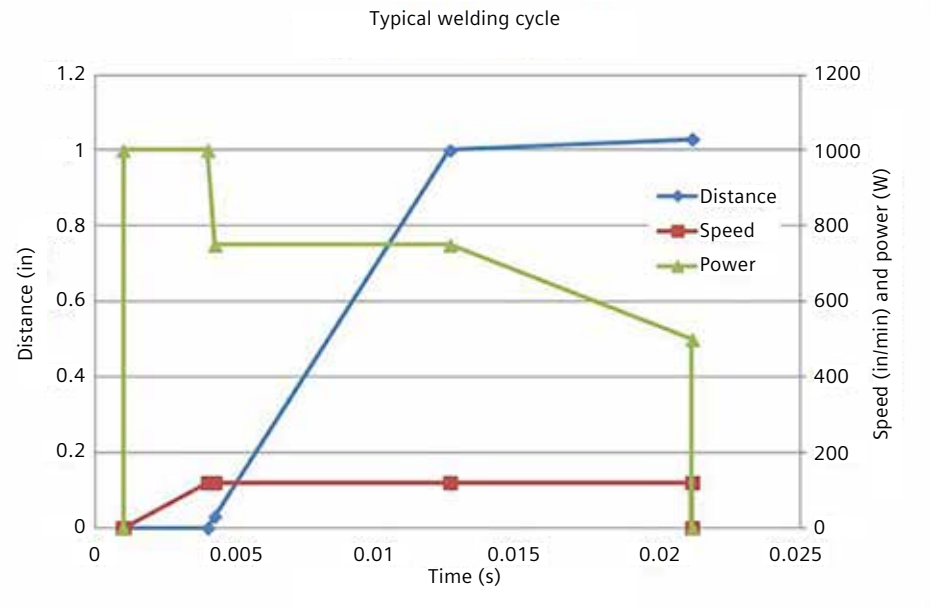


Figure 2: Typical welding cycle.

and high-value component parts was prohibitively expensive and time consuming. It was obvious that simulation was the answer. But high-fidelity simulation of the complete keyhole physics was complex, expensive and slow. The simulation had to adequately predict quantities of interest – such as weld pool diameter and zone shape as well as penetration depth – in order to specify the optimal laser process parameters.

Seeking a solution

Contemplating the task at hand, Bemis recalls, "We needed an economical solution – one that was fast, robust and easy to use." In search of this solution, he spoke with his support engineer at Siemens Digital Industries Software, who had experience simulating welding. Based on the guidance he decided to use Simcenter STAR-CCM+ to conduct the simulations.

Simcenter STAR-CCM+ features a comprehensive suite of geometry creation and preparation tools that significantly reduce the number of man-hours required to prepare a model for meshing. In addition, Simcenter STAR-CCM+ features a single integrated environment, which provides a fast, most

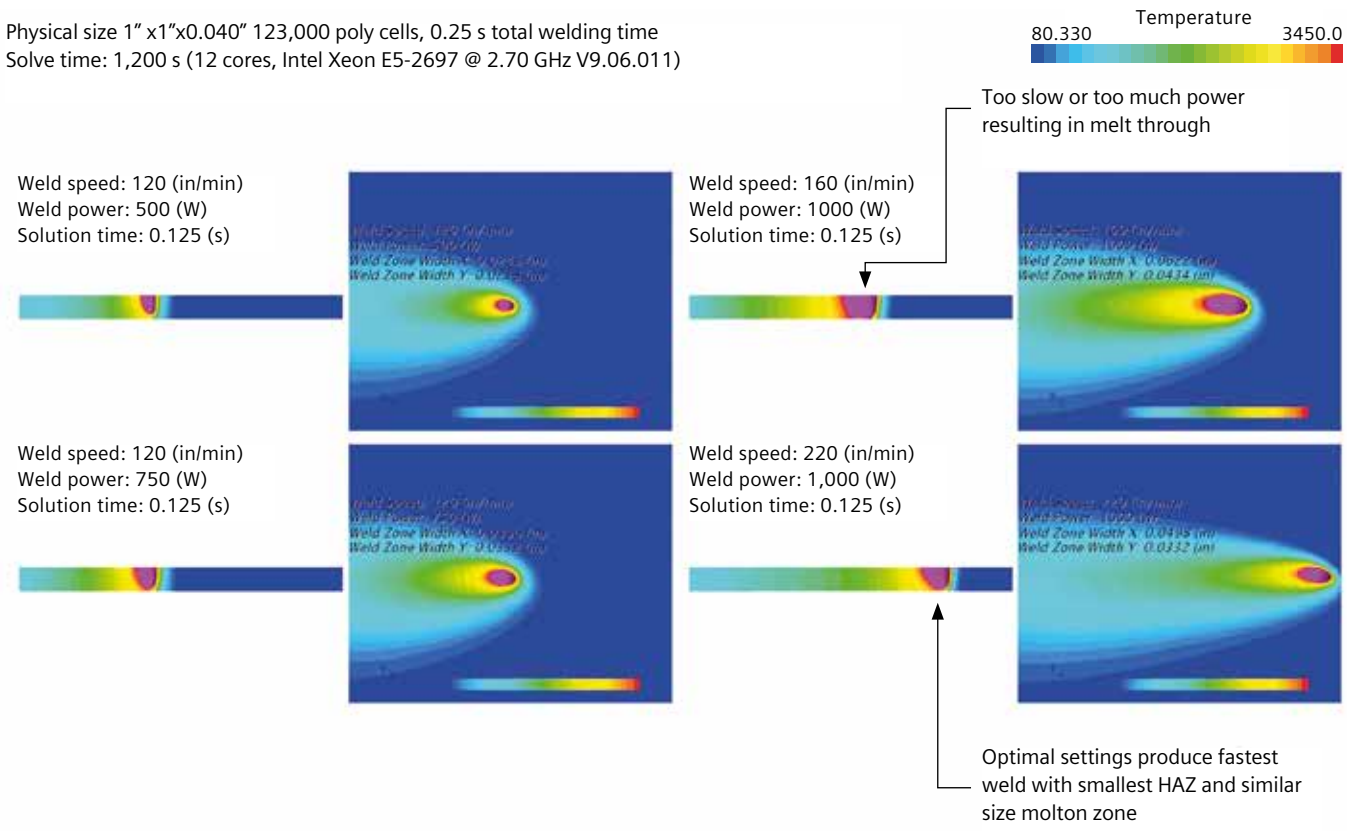


Figure 3: One of the MDX concepts that Bemis employed to design the component was an add-on module known as Simcenter STAR-CCM+ / Optimate.

automatic route from complex CAD models to engineering solution. This met two of Bemis' main criteria: speed and robustness. As to ease of use, the software's powerful meshing tools cut down geometry preparation and meshing time from weeks and months to hours, while delivering a high-quality mesh on sophisticated geometries. All of these capabilities can be leveraged from within familiar computer-aided design (CAD) and product lifecycle management (PLM) environments. Bemis used Simcenter STAR-CCM+ to simulate the welding heat transfer process. The solution proved to be excellent in predicting both the weld width and the behavior of features affected by the blind welding. "Simcenter STAR-CCM+ has the unique ability to simulate the welding process and provide insight into the thermal transient experienced during welding in a manner that is both practical and fast enough for industrial use," Bemis says.

Power of overset meshing

For the past 30 years, engineers trying to perform computational fluid dynamics (CFD) simulations struggled with the interaction between multiple moving objects. Traditionally, this required the generation of an interconnected mesh between the objects, an intensive manual process that was extremely difficult and time consuming. In fact, it was almost impossible if extreme ranges of motion or close interaction between objects was involved.

With overset mesh, Simcenter STAR-CCM+ solved the problem. Overset meshing, sometimes called overlapping or chimera mesh, in Simcenter STAR-CCM+ presents a new and more effective way to handle the modeling and simulation of the complex physics associated with moving objects. This approach allows the user to generate an individual mesh around each moving object, which can then be moved at will over a background mesh. "In the welding process, you can either move the heat source or the material," Bemis says. "Overset meshing allows you to simulate the relative motion between the heat source and the parts that are being welded together. That motion, along with the laser's power,

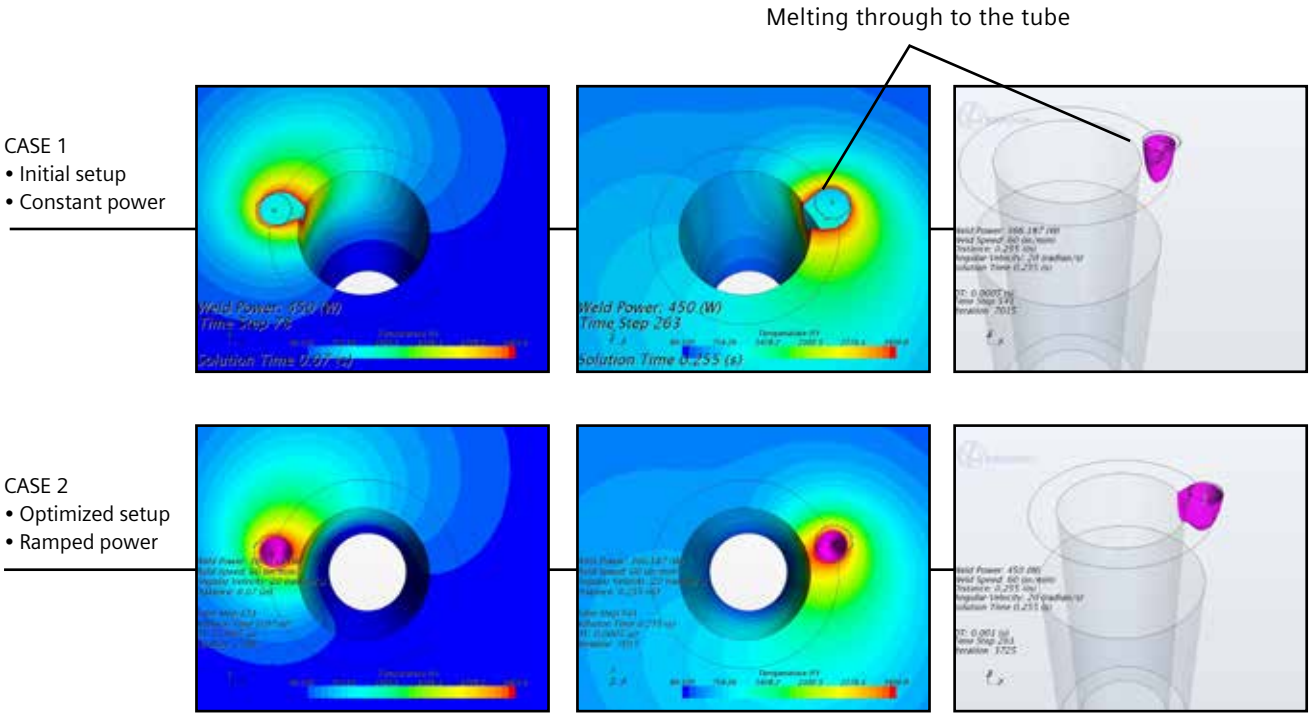


Figure 4: Optimized start dwell and ramp produces a full depth weld at the start. Decreasing power ramp through the circular weld maintains weld size and depth as heat builds up.

really dictates how wide the weld gets, the size of the molten zone and the depth of penetration. With the use of overset meshes, we were able to run a fairly coarse background mesh as well as a fine, detailed mesh of the weld zone. We moved rather arbitrarily through the background mesh and generated any weld pattern we wanted. Some of the welds were 100 mm long and ½ mm thick, resulting in big aspect ratios and a really large mesh count to refine the simulation in the weld zone areas."

Bemis was working with a moving target. Heat tends to build up in the weld zones, resulting in changing parameters as you move from weld to weld. Overset meshing allows the designer to simulate individual welds on the component, taking into consideration the changing nature of the material being worked on due to heat transfer. An implicit unsteady simulation with a moving overset mesh permits the prediction of the extent of the molten zone as it progresses along the joint, temperatures in the work piece and heat transfer to the fixture.

Parameters such as laser power, travel speed, acceleration and pulse frequency can be tuned to provide the desired optimal weld.

A new methodology

The research team also worked with a methodology known as Multidisciplinary Design eXploration (MDX). MDX allows the automatic testing of designs from early in the concept stage against all of the physics that might impact performance. This is possible because the increasing capabilities of sophisticated simulation software such as Simcenter STAR-CCM+ allow engineers to determine how a product will perform under the conditions it will face during its life cycle.

"We used Optimate to explore the parameter space up front and alter the process and components to get the final results we wanted," Bemis explains. "We were able to set up weld speed, power and field functions to mimic laser control. We could ramp the laser up and down, simulate voltage feeds, and all the other parameters that Optimate could access. We then used the software to run

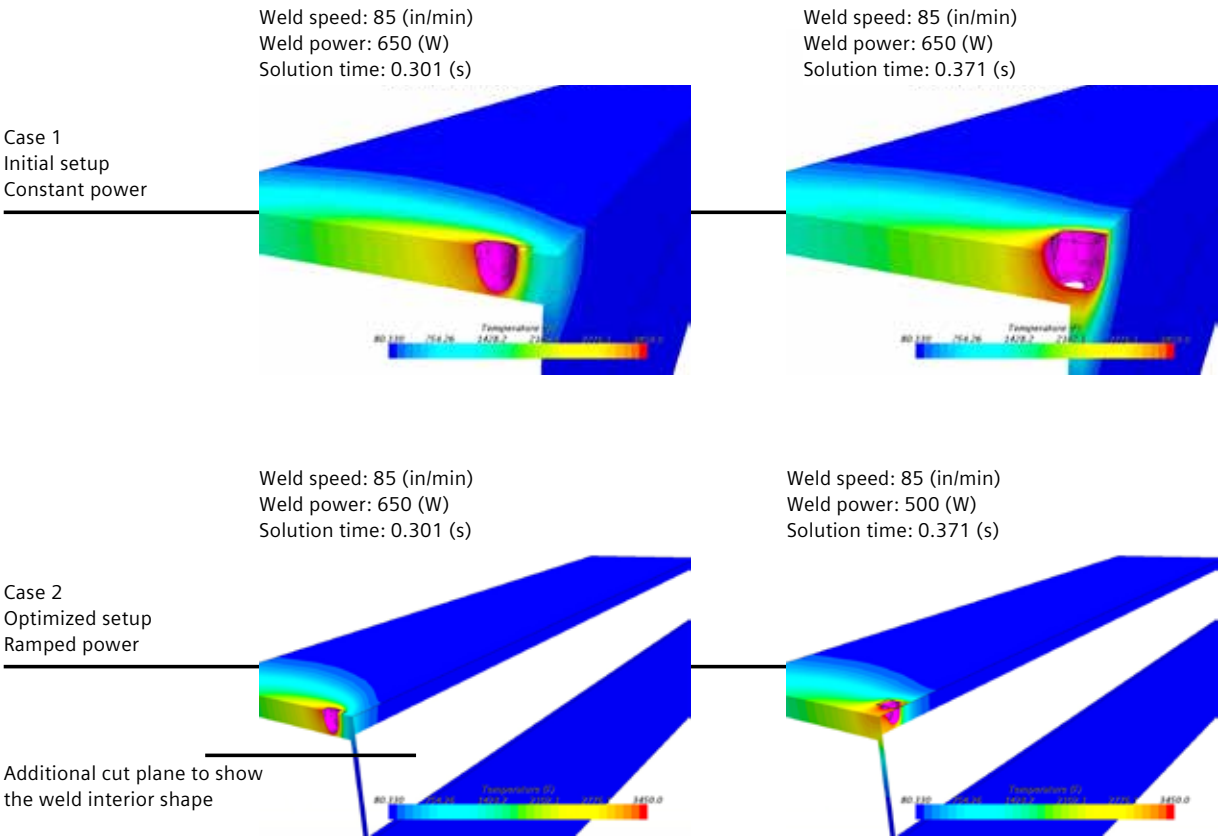


Figure 5: Case 1 shows how weld pool melts through the corner at constant power and speed. Case 2 pictures an optimized setting allowing for a uniform melt pool throughout the weld cycle.

cases to determine such things as how far back from a corner we needed to slow down, and how much to drop laser power in order to make a weld around a sharp corner while maintaining the same heat effective zone in the base material components. The simulation allowed us to prescribe all the welding parameters for experimental validation early in the design process."

"Accurate enough"

He points out that using the Simcenter STAR-CCM+ simulation solutions meant that the results were "accurate enough." Rather than attempting to generate a perfect simulation of the problem, the results they obtained provided sufficient information to accurately predict real world weld characteristics, evaluate parameters and decide which directions to take. This process, Bemis says, was very fast considering it was a fully transient simulation with motion and overset meshing. He was able to run enough cases on a high-end workstation loaded with Simcenter STAR-CCM+ / Optimate to allow design space experimentation and optimization. The software is flexible enough to simulate complex motion in time-dependent parameters for a heat input field function interface. "It's incredible to have that kind of power at your fingertips without having to write your own C code or FORTRAN," Bemis explains. "I figure we saved at least six months of trial-and-error development – six months of experimental lab time – which is huge. In fact,

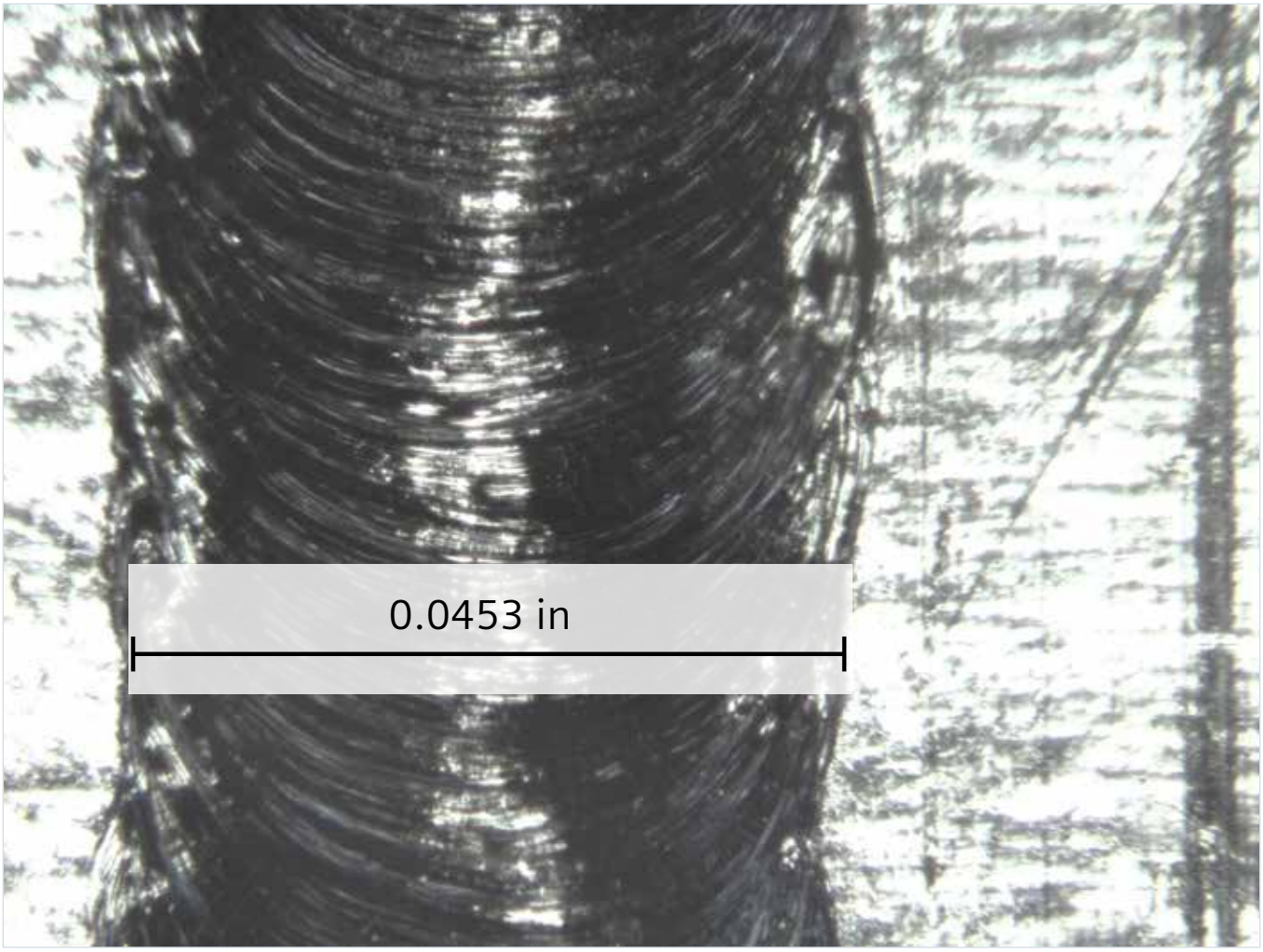


Figure 6: Validation of weld zone width and depth was done using optical microcopy.

by freeing up more time for design, we managed to figure out how to avoid using blind welds, a definite plus. The high quality simulation using Simcenter STAR-CCM+ and Optimate allowed us to explore the research, design and analysis of the component as well as the manufacturing process all at the same time. We were able to deliver the final component design to our manufacturing facility complete with all the fab steps and processes in place. This is a very powerful way to work.

"We use Simcenter STAR-CCM+ every day. The software has become an integral part of our design and development activities."

Reference

Praxair Direct: Welding Terms Glossary

JFE techno-research mobilizes simulation for Japanese-style manufacturing

Toshiki Hiruta, director of the CAE Center.

Joji Kato (center) with Katsuhiro Iwasaki (left) and Norikazu Sato (right).

The role of JFE techno-research within the JFE group

JFE Steel Corporation, a company that has been in the industry for more than 100 years, boasts the world's fifth-largest scale in terms of its crude steel production. JFE Techno-Research Corporation, a member of the JFE Group, undertakes fluid analysis, structural analysis and other areas of the JFE business, including evaluation, investigation and examination of materials. They cater to steel plants, environmental engineering and other areas within the group, and are also actively contracting for business outside the group. In particular, it undertakes engineering service projects from diverse industry areas, including automobile, machinery, electrical machinery, electronic components, construction and civil engineering and research institutions. They are providing engineering solutions and consulting services for these areas based on highly reliable analysis and evaluation technologies.

JFE Techno-Research focuses on the following two areas:

1. The ability to propose solutions not only based on analysis, but also based on experience cultivated over many years in the steel industry

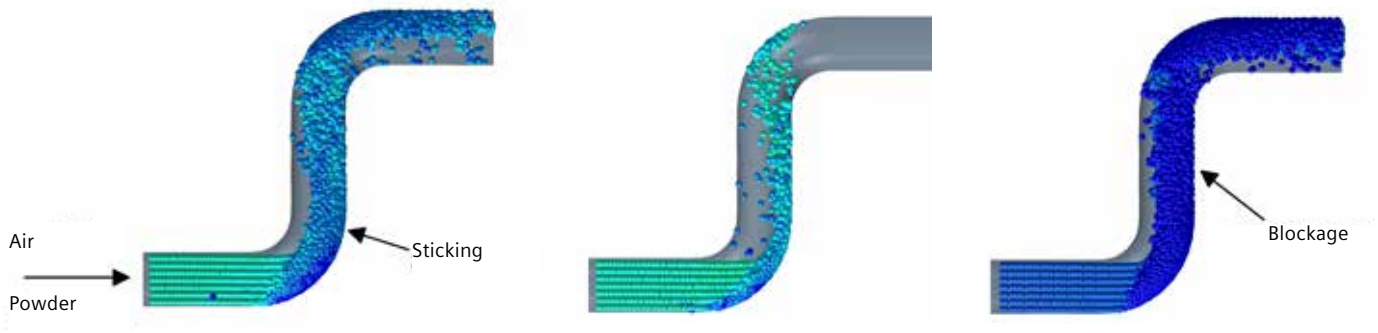


Figure 1: Powder behavior analysis in powder transport piping using Simcenter STAR-CCM+.

2. The packaging of proposals with testing results: The Solution Division (Kawasaki) is comprised of the CAE Center, the Sensing and Visualization Analysis Center, Structure Performance Department, Material Performance Evaluation Department, Equipment and Process Technology Department and other specialized testing and analysis divisions, providing a full suite of services.

JFE Techno-Research offers interpretation of analysis results, guidelines for design improvements and consulting related to all aspects of "Monodzukuri" (Japanese-style manufacturing), which helps stabilize product quality and reduce production costs. In this article,: we talk with members of the CAE Center at JFE Techno-Research about the crucial role of numerical analysis in Monodzukuri.

Improvements in calculation accuracy: Partnering with the measuring division for verification

The single greatest challenge in engineering simulation is the verification of the numerical results. Correlation of numerical analysis with physical testing improves the accuracy of the final results. The target in normal flow analysis at JFE is an accuracy of ±3 percent when compared to test results. However, for more complex models that include chemical reactions, multiphase flow and other phenomena, the analysis accuracy typically swells to around ±10 percent. Toshiki Hiruta, director of the CAE Center, noted that "while our target is ±3 percent, with staffers who have built up a certain degree of experience, it becomes reasonably possible to tell whether or not the outcome is appropriate by examining the results."

Senior research engineer Katsuhiro Iwasaki offered the following comments: "Depending on the customer, in some cases we receive requests for both testing and analysis. This actually presents a rather stiff challenge, and because we come up with test values, there is a need to adjust with the analysis results at the next stage. This is particularly true as the analysis grows more complex, which proportionally raises the importance of interpreting the test values and running comparisons against the analysis results. There are also cases in which our customers present us with test results, asking us for customization based on the models suggested by those results."

At JFE Techno-Research, the merits of operating measuring divisions are utilized with regard to CFD in taking actual measurements of temperature, flow velocity, gas composition and other parameters. That data is then compared to the CFD results to verify its soundness and further improve the accuracy of the outcome. Figures 1 to 3 show some application areas of simulation at JFE Techno-Research: powder behavior analysis in powder transport piping, cast part fluidity and solidification analysis and hydrogen leak diffusion behavior analysis.

Addressing diverse CFD challenges: From single phase to multiphase flow

For the CFD-related operations at the CAE Center, Iwasaki is in charge of simulations for chemical reactions, combustion, explosions and other thermofluid process issues. In addition to that work, he also engages in support, RandD on his own initiative and other tasks that range from basic research to the creation of machinery. Deputy general manager Norikazu Sato meanwhile serves as the CFD technology staff member primarily devoted to multiphase flow analysis involving thermofluids, heat transfer and particles, and other duties. Hiruta outlines the role and analysis themes of simulation at the CAE Center: "The work here involves various fields but the core of our operations lie in undertaking projects related to structures, fluids and fluid-structure interaction (FSI) analysis. In addition to: the aforementioned tasks, the CAE Center is also active in the development of analysis methods for application in new fields. In fluid analysis as well, for example, RandD is being advanced not only on a single phenomenon basis, but also geared to more complex phenomena known as multiphysics. While the company includes a division that develops its own numerical simulation code, it also utilizes commercial CFD software to expand the fields of adaptation." JFE Techno-Research and Siemens Digital Industries Software are collaborating on building models to support such RandD efforts.

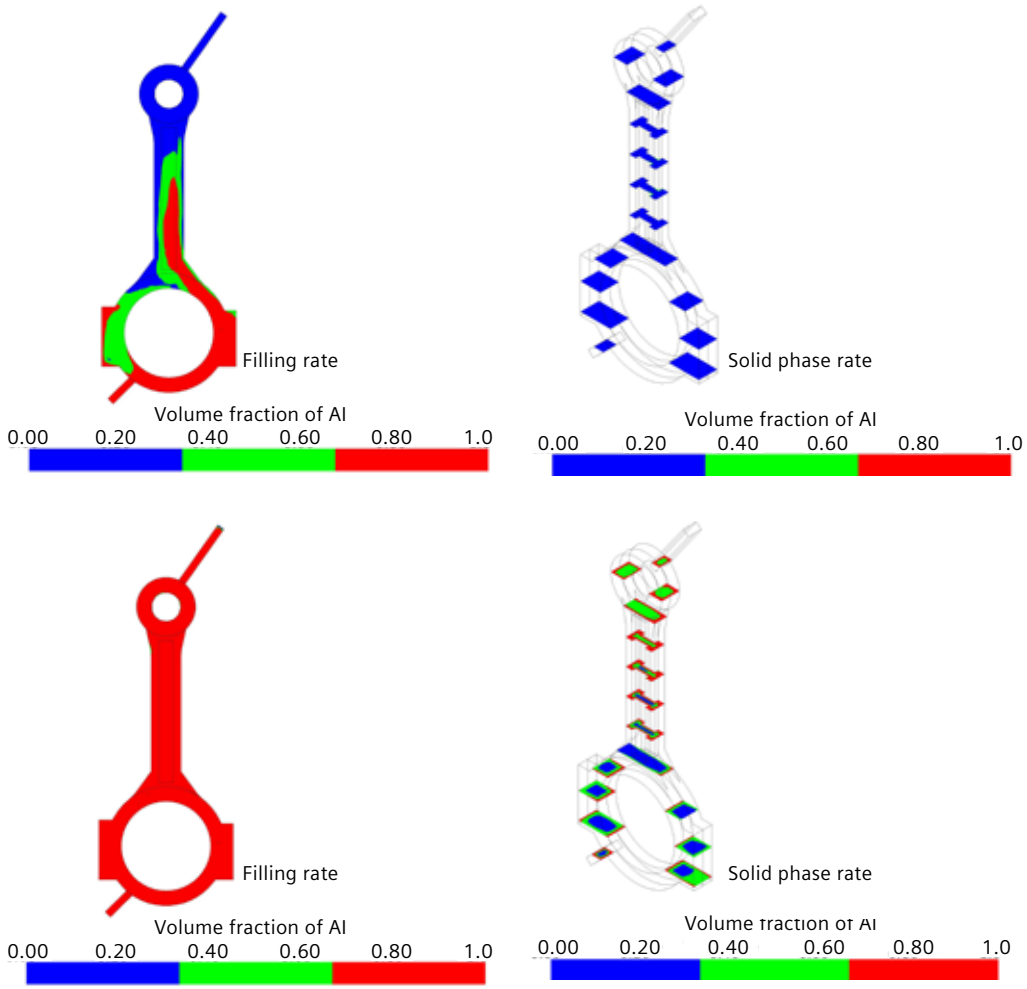


Figure 2: Cast part fluidity and solidification analysis using Simcenter STAR-CCM+ showing filling rate and solid phase rate during casting (above) and post-casting solidification (below).

The importance of interpretation and evaluation of analysis results

Sato explains the system used to implement the analysis operations: "Our center has acquired certification under ISO 9001 as our quality management system (QMS). In performing analysis, we assign project managers to each engineering service project, effectively deploying a check system to ensure that the analysis is conducted correctly and in keeping with the specs. In most cases, the standard approach is for one technical staff member to serve as the project manager, with one or two younger team members performing the actual analysis. While it is the young staffers who work with the CFD code to advance the work, depending on the specific analysis, there are also cases when senior engineers step in to operate the analysis software, perform customization, test calculations and other tasks." Next, we inquired about the key points of care when undertaking analysis as a team, means of sharing information between the company's various departments/locations and other relevant challenges. Iwasaki explains the methods of communication: "We devote particularly keen attention to maintaining close connections in our reporting, liaison and consultations, as well as preserving confidentiality. It is desirable, meanwhile, that on-the-Job-training (OJT) for our younger team members be effective in simultaneously raising their potential and passing on the company's technology. Without effective reciprocal communication, we run the risk of moving in different directions and perpetrating irreparable mistakes."

He continues: "When implementing analysis on the foundation of stipulated conditions or assumptions, we also hypothesize questions likely to be voiced by the customer regarding the viability of the results and advance the work while sharing ideas with our young team members. In the area of model building, I sense a vital need to engage in close reciprocal communication with our younger people in working to determine if our results appropriately reflect the technical concepts of the analysis targets, how to evaluate the analysis results and how to explain the outcome to

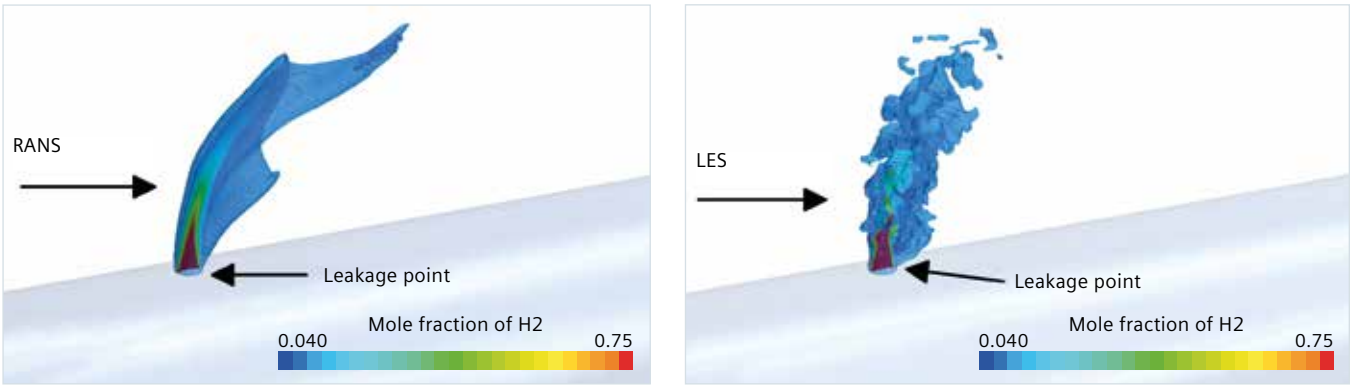


Figure 3: Hydrogen leak diffusion analysis using RANS (left) and LES (right) in Simcenter STAR-CCM+.

customers. In particular, due to the fact that it usually proves unfeasible to fully simulate the actual physical phenomena, chemical reaction processes or other conditions with CFD, we devote special care to the methods of hypothesis and projection, as well as to the interpretation and evaluation of the results of our analysis. For our young members, I set aside particular time and attention to stress the importance of grasping what the customer wants to learn, what they truly have in mind and other key concerns."

Hiruta adds: "When we undertake consigned analysis projects from our customers, our teams perform the analysis and write reports. My mission is the final confirmation of the reports. The most important thing in the process is to consider how to raise the quality of our future analysis in cases when the results fail to measure up to the customer's expectations. Meanwhile, while it is naturally important to examine the results, it remains extremely tough to perform such severe reviews on the analysis results alone."

Simcenter STAR-CCM+ offers high hopes for expandability above and beyond CFD

At JFE Techno-Research, Simcenter STAR-CCM+ has received stellar evaluations on two key points. First, the integrated workflow, which spans geometry preparation, meshing, physical modeling, analysis and postprocessing, is considered extremely user-friendly. Secondly, the multidisciplinary software package provides linear stress analysis options both within the code and through coupling to Abaqus and other stress solvers, facilitating its use in evaluations of material selection. Looking ahead, there are also high hopes the addition of FEM functions from v10.04 onwards will further expand the FSI analysis domain.

According to Sato, Simcenter STAR-CCM+ has earned solid accolades for truly shining in terms of its meshing function: notably, the ability to create a mesh with simple operations even when working with rather complex geometries. He says this is the key to swift analysis of prototypes. Sato also praised Simcenter STAR-CCM+ for being able to readily link up multiple physical models, easy customization via field functions and scripting, and other advantages.

Finally, we asked about the enhancements they would like to see in Simcenter STAR-CCM+ and Siemens services. Iwasaki is conducting studies and evaluations on the streamlining of a simplified manufacturing process simulation independently with Simcenter STAR-CCM+.

He wants to output the cooling speed with solidification analysis, distribution of secondary phase in dispersion strengthened material, and let them be reflected in material properties. Iwasaki believes that if the fruits of these efforts can be channeled back to Simcenter STAR-CCM+ for performing linear stress analysis finding stress concentration area, it should be possible to realize more efficient shapes and processes. Sato is advancing work on analysis proposals and engineering services in the areas of DEM, FSI, large-scale computing and optimization. With Simcenter STAR-CCM+ offering a high level of customization, he believes it will be possible to propose complex analysis techniques at a truly unprecedented level. Hiruta also mentioned potential applications in healthcare-related fields – with particularly efforts currently being channeled into the implant structure analysis realm. He also admits that while fluid analysis in life sciences remains a largely unknown domain, it is nevertheless a challenging area for growth.

Conclusion

The CAE Center in JFE Techno-Research is undertaking a considerable number of projects outside of the JFE Group. The reports of how they are using their CAE experience in other fields is inspiring. Hereafter, in addition to the CFD analyses, they will deal with the FSI analysis and new fields such as healthcare. Siemens certainly stands ready to mobilize the full span of its global resources in doing everything possible to support their efforts.

Mixing industry: Saving with fine-tuning or design exploration?

Introduction

Mixing, the art of transforming a set of components into a homogenous product by blending them together, plays a critical role in many chemical processes and pharmaceutical applications. Think about all the products you use in your daily life and picture how paralyzed our industries and consequently our lives would be without mixing. From food in grocery stores, healthcare and pharmaceutical products to polymers, minerals, paint and coating, biofuels and many others, most products require mixing as a crucial production step. For industries to deliver a uniform blend of a desired weight/volume with consistent particle size distribution, color, texture, reactivity or any other required attributes, and to avoid the high cost of penalties associated with poor mixing, it is critical to control the quality of mixing.

In addition to eliminating the costs associated with the operation of deficient systems, there is a pressing need for product improvements, making it critical to find the best strategies for achieving faster blend times and increased mixing quality with minimal investment and operating costs. With the help of advanced simulation and optimization software, there is no longer a need to take the conventional route of trial and error to achieve the best design. Once engineers identify the important mixing performance parameters, they are now able to simulate hundreds of design points quickly to pinpoint the best design to increase efficiency of the system and gain a competitive advantage.

Stirred tank design optimization study

Typically, for a generic stirred tank reactor, the design objectives are mixing time, mixing quality and power consumption. These objectives need to reach a minimum, maximum and a specific value, respectively. In order to achieve these objectives, improvements are required on many aspects of the design process, including mechanical, electrical and chemical components. From the mechanical perspective, the design parameters could be in impeller configuration, vessel size, vessel type, number of baffles, etc. One core issue for this type of optimization problem is there is a nonlinear relationship between design parameters and design objectives, which makes the design modification a time consuming and tedious job. If design engineers need to make improvements by prototyping the new system at laboratory scale, and subsequently scaling it up to production capacity, it becomes a costly and time-consuming process. This is where using numerical design optimization adds great value, as it allows for autonomously making subtle improvements to the design parameters to generate an optimal stirred reactor before physical prototypes are even built. Numerical mixer optimization should be seen as a decisive business tool that can fulfill profitability requirements, resulting in a significant competitive advantage while delivering a better quality product.

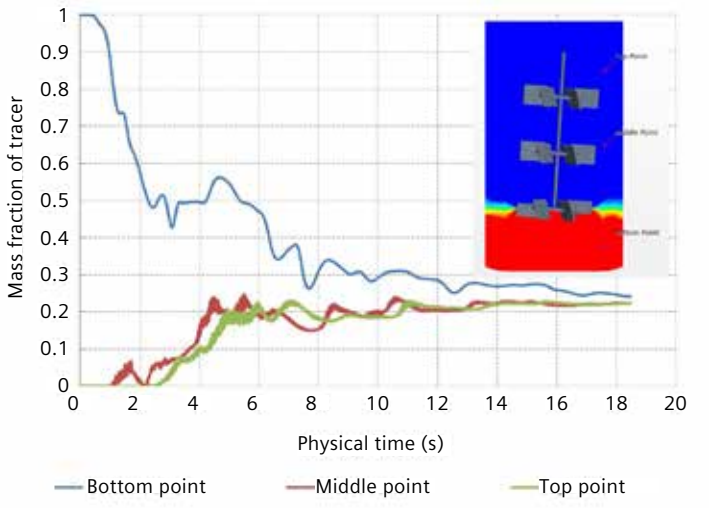


Figure 1A: Inert tracer method (resembling the widely used experimental technique) showing the quantitative change in local concentration as a function of time.

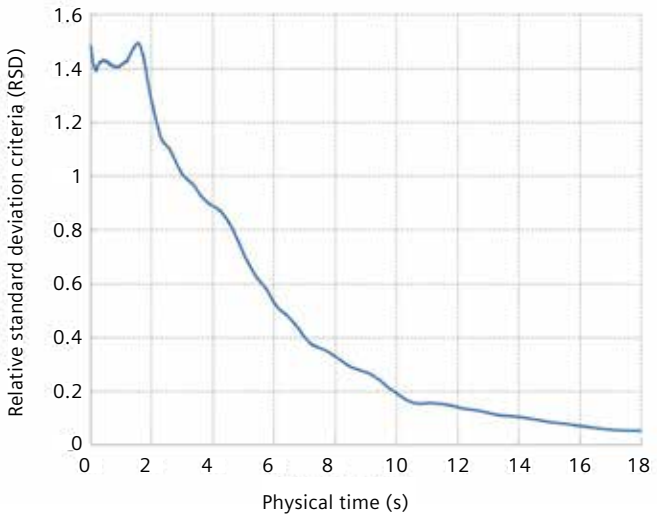


Figure 1B: Relative standard deviation method.

It is noteworthy that often, for the optimization studies, the objectives are competitive in nature and thus, there is no single optimum design. For instance, if a mixer design engineer is to both minimize the mixing time and minimize the power consumption, there would be no design that offers the best value for both objectives. An improvement in mixing time can be obtained only by sacrificing the power consumption. In such scenarios, a nondominated sorting algorithm finds the design that is best in terms of one objective for a given value of the opposing objective. The result of a Pareto optimization study is a set of designs that satisfy this condition, which is also referred to as the nondominated design condition.

In this study, a series of tuning parameters for a stirred tank design along with two competitive objectives were identified:

1. Power number versus mixing time.

2. Impeller moment versus mixing quality.

The main goal was to find an optimal tradeoff between the competitive objectives for each case. In this regard, a multi-objective mixing study has been carried out for mixing using MO-SHERPA, which is a set of Pareto optimum designs. Before plunging into the numerical approach, we need to first identify the mixing criteria will be addressed in the following section.

Mixing criteria

The mixing time can be defined as the time it takes to achieve a predefined level of homogeneity in the mixture. It can be difficult to identify the best approach to quantify mixing in terms of time and quality. There are several experimental methods to evaluate the mixing quality such as decolorization, electrical conductivity and pH measurements. However, all of these methods are accompanied by uncertainties as they are based on injecting a tracer into the mixture and then measuring its concentration either visually or with probes at various locations. For instance, the mixing time required to obtain 90 percent homogeneity is the time needed for the fluctuations of the tracer concentration to be less than 10 percent of the concentration would have been achieved with perfect mixing. However, studies have shown that this value can be significantly affected by the probe size or tracer injection location. In addition, these methods only give an indication of the mixing quality at a limited number of probe locations, and thus a larger number of sample points are required to get a more accurate picture, which is tedious, time-consuming and costly. This shortcoming can be easily addressed using numerical techniques, and the best approach is to use statistical analysis on the quality of mixing at every cell inside the numerical domain. In this regard, Simcenter STAR-CCM+

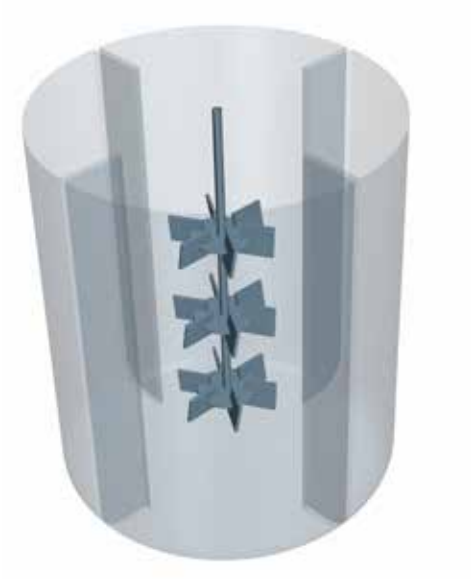


Figure 2A: Mixing tank geometry created in Simcenter STAR-CCM+.

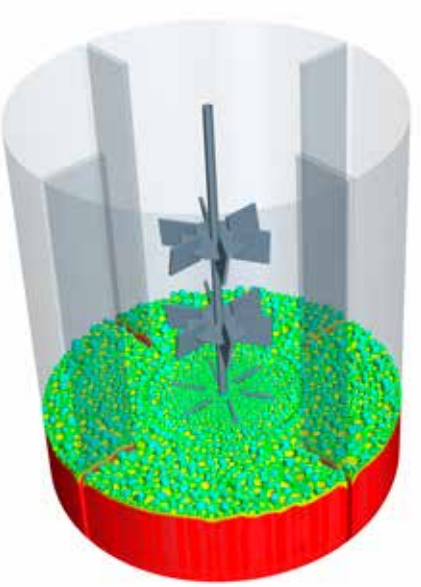


Figure 2B: The initial condition of tracers defined by field function.

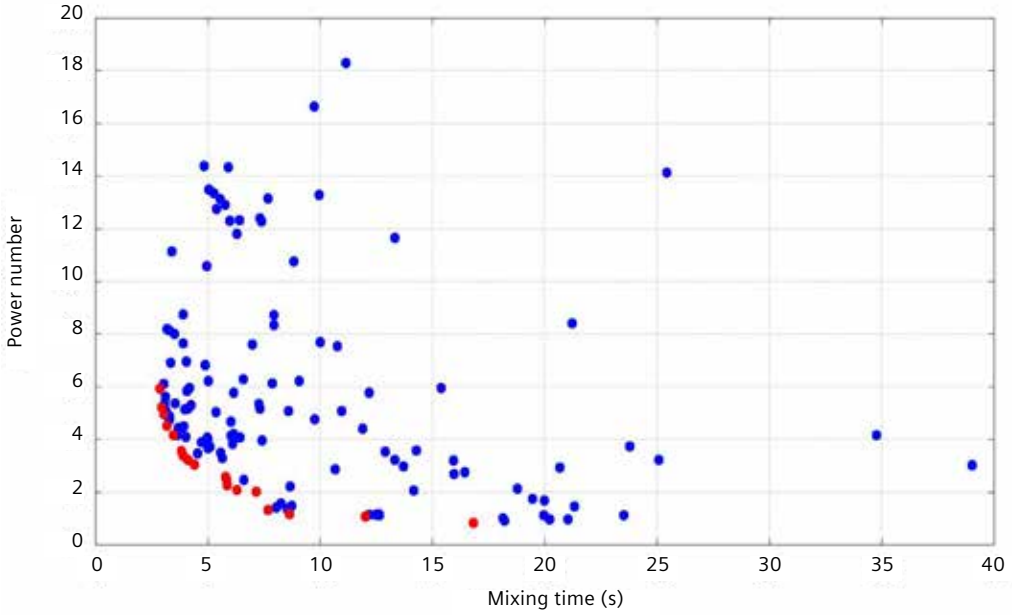
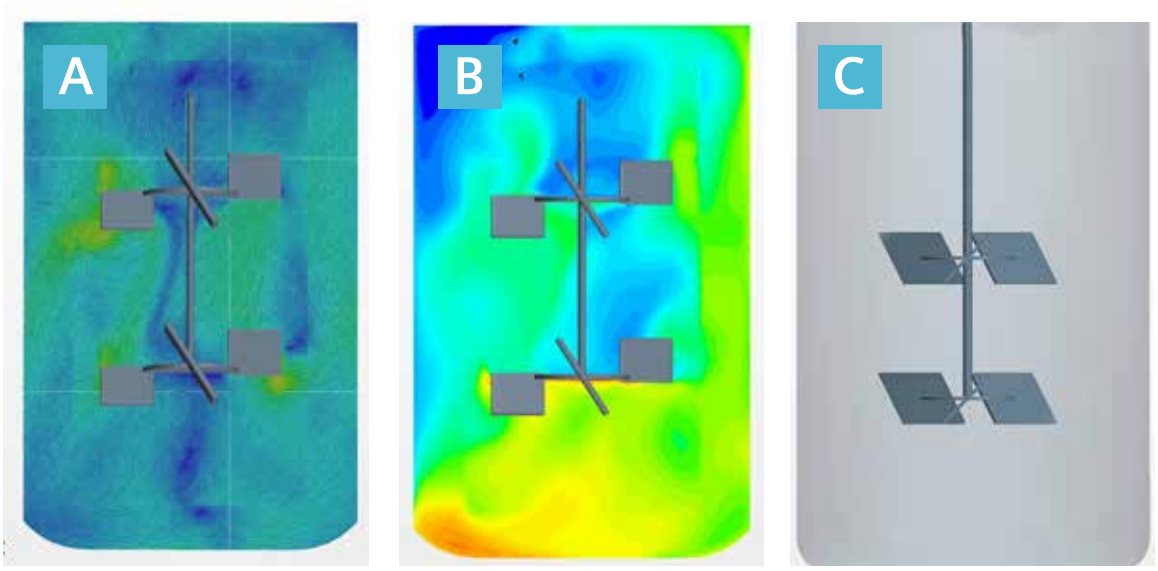


Figure 3: The results of Pareto front (red dots) show the designs forced by the optimizer to the optimal corner.

has the capability of defining a variety of desired mathematical formulations for measuring the mixing quality through field functions. Also, Simcenter STAR-CCM+ allows us to define a homogeneity threshold, which permits the user to visualize poor mixing areas over the mixing cycle.

One of the numerical techniques that can be used for assessing the quality of mixing is the relative standard deviation (RSD) method, which is the ratio of standard deviation of the tracer's mass fraction over the entire domain to its corresponding average concentration. RSD can be formulated as follows:



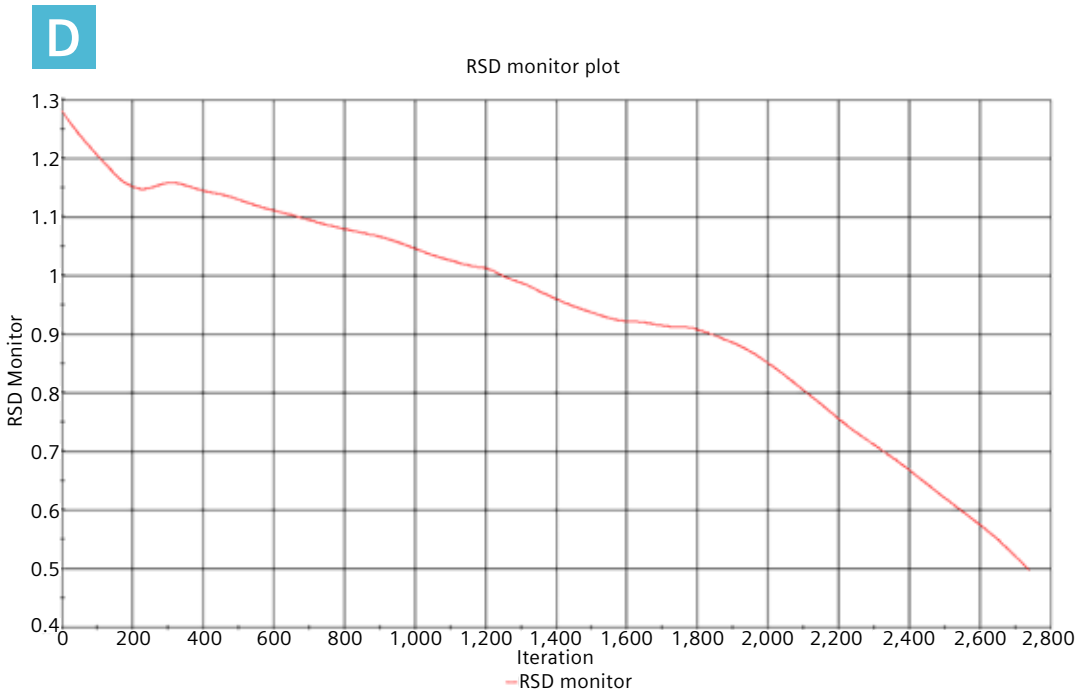


Figure 4: Velocity field (A), Tracer's mass fraction (B), CAD geometry (C) and RSD vs time (D) for one of the design points on the Pareto front.

$$RSD = \frac{\sigma}{\bar{C}} \quad \text{where} \quad \sigma = \sqrt{\frac{\sum_{i=1}^{n}(C_i - \bar{C}}{n-1}}$$

Where Ci is the mass fraction of the tracer at the i^{th}cell, C is the volume-averaged value of mass fraction of the tracer in the entire domain, and n is the number of cells. Good mixing corresponds to a low RSD value. Figure 1 shows a comparison between the inert tracer method (1A), which resembles the traditional experimental technique, and the RSD method (1B), both using Simcenter

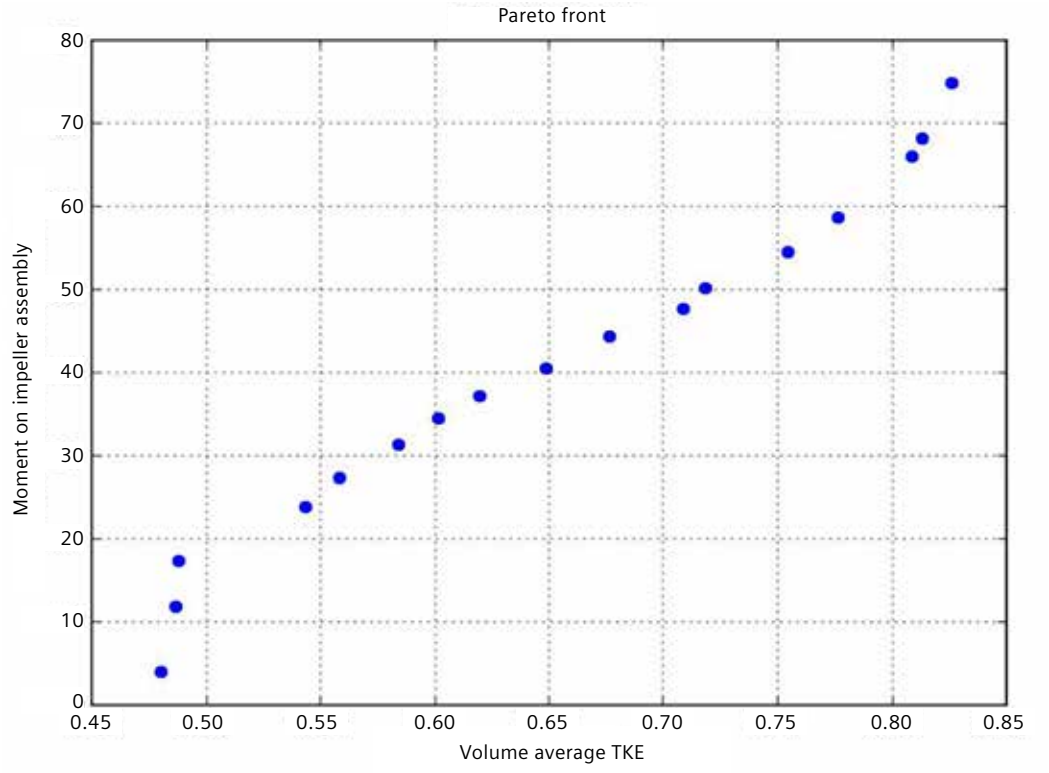


Figure 5: Pareto front for the moment on the impeller assembly versus the volume-averaged TKE.

STAR-CCM+. As can be seen, the experimental method keeps track of the quantitative change in local concentration as a function of time, while RSD guarantees the quality of mixing over the entire domain. Thus, RSD can address the issue of the experimental approaches being spatially biased. This is one of the significant advantages of CFD over experimentation.

In this study, the mixing quality is quantified using the RSD approach and the mixing time is defined as the time it takes to reach an RSD value of 0.3, which does not denote ideal mixing, but serves as a common value for good mixing.

Numerical approach

The parametric mixing tank geometry was created in Simcenter STAR-CCM+ using the 3D CAD modeler (figure 2A). Mixed liquid was tracked as a passive scalar that is initially at rest at the bottom of the tank (figure 2B). A transient simulation was performed using the moving reference frame (MRF) approach. Here, the two competitive objectives being 1) power number versus mixing time, and 2) impeller momentversus mixing quality are discussed.

Competitive objectives 1: power number versus mixing time

Advanced CAD modeling capabilities in Simcenter STAR-CCM+ allow users to define any design characteristic as a parametric variable, which can then be used as an input variable for optimization with Optimate. In this study, seven design variables were chosen for the optimization:

- Number of impellers (2/4/3)
- Number of blades per impeller (3/9/7)
- Impeller blade angle (0/45/16)
- Impeller blade height (0.01/0.06/11)
- Impeller radius fraction (0.2/0.5/21)
- Number of baffles (2/6/5)
- Baffle height fraction (0.6/1/21)

The three numbers in (a/b/c) format show the starting point, the number of divisions for increasing the parameter, and the end point. In addition to number of divisions, Optimate has the choice for specifying the increment. For example, the increment for the number of impellers would be 1 (minimum=2, maximum=4, increment=1). Both methods define the range within which the variables can be fine-tuned in Optimate. In this study, this

number corresponds to a total of 8,149,680 variations. Covering this design space manually would be nearly impossible. Instead of running over 8 million design points, Optimate uses the Sherpa optimization algorithm that can reduce the number of evaluations to a time efficient number of runs per design variable. This algorithm learns as it goes along and it modifies its strategy to most effectively search the design space, giving a significantly reduced number of runs while still likely to come up with a better answer. In this case story, it took Optimate only a few days to search the design space, and complete hundreds of evaluations for the best results. The first set of optimization objectives was defined as follows:

- Minimize the power number
- Minimize the mixing time

The set of outcomes resulting from the optimization is called the Pareto front. In figure 3 the clustering of dots close to the Pareto front illustrates how the optimizer is forcing the designs towards the optimal corner, which corresponds to lower values of mixing time and power numbers. This plot answers questions such as, “What is the minimum possible power number for a specific mixing time?” or “For a specified power number, what is the minimum possible mixing time?” These are questions that are worth millions of dollars in the mixing industry. Figure 4 shows an example of CAD design, tracer’s mass fraction and a RSD-time plot as calculated by Optimate for one of the design points.

Competitive objectives 2: impeller moment versus mixing quality

In order to study this objective, the following parameters were considered:

- Number of impellers (1/5/5)
- Impeller blade angle (0/90/19)
- Number of baffles (0/9/10)
- Baffle height (0.005 m/0.012 m/15)

It should be noted that depending on the user’s objective, different variables can be specified.

The optimization objectives were as follows:

- Maximize the volume-averaged Turbulent Kinetic Energy (TKE)
- Minimize the moment on the impeller assembly

The Pareto front (figure 5) shows the designs for which the maximum possible volume-averaged TKE is reached for a given moment on the impeller assembly.

Conclusion

Stirred tank design engineers have always been driven by the desire to reach the highest mixing efficiency, which is influenced by competitive objectives such as mixing time versus power consumption, or moment on the impeller assembly versus turbulent kinetic energy. Because these objectives depend significantly on the geometry of the tank and the impeller, a multi-objective parametric study is required to identify the best design that could dominate in both objectives.

Simcenter STAR-CCM+ offers SHERPA, a robust hybrid algorithm-based optimization method provided by the Optimate plugin, which allows for the investigation of a large design space in a short amount of time. After validating the baseline simulation against experimental data, performing the optimization study provides the best design for a predefined set of operating conditions, ultimately resulting in savings worth millions of dollars.

The Pareto front plot can provide the answer to the mixing industry's million dollar questions such as, "What is the minimum power number possible for a specific mixing time?" or "For a specified power number, what is the minimum mixing time possible?"

Simcenter STAR-CCM+ provides Pierre Guerin with a competitive edge

Introduction

Like many successful entrepreneurs, Pierre Guerin started by founding a small family The business, which was started in 1949, had five employees and was involved in agricultural and dairy maintenance equipment. It took decades of evolution of products, brands, contributions and innovations to turn his startup into a successful corporation, which is now recognized as the major European supplier of stainless steel process mixing vessels for the chemical/food/beverage and pharmaceutical industries. For these industries, mixing is a key unit operation as the quality of products is highly dependent on how effectively and efficiently the components with different properties mix with each other in order to reach a uniform blend with the desired attributes.

For Pierre Guerin to maintain its competitive advantage in the market, it is crucial they design and manufacture equipment that guarantees the highest level of mixing quality while keeping operational time and cost as low as possible for its customers. In this case, it has never been easy to take a traditional scale-up approach from lab scale to production. It involves time consuming and expensive experimentations to test and verify any new ideas during the design process. CFD simulations provide a robust tool for modeling the system to plant scale that also captures all the key physics and required quantities in continuum space, explores the design space faster, and hence reduces the number of trials required for optimization of stirred tanks. In this way, engineers are able to submit only the most promising design to physical testing. In mixing vessel applications, some of the main targeted characteristics are the pumping number, the power number and the mixing time. In order to select the most efficient CFD tool to predict these numbers, mixing engineers at Pierre Guerin conducted validation studies using several CFD software tools, including Simcenter STAR-CCM+.

This article outlines the comparison between the numerical results of Simcenter STAR-CCM+ and experiments carried out to validate the behavior of the company's patented propeller. A similar validation study on a Rushton turbine has also been performed and documented [1].

Geometry and mesh

Simcenter STAR-CCM+ can be used to model different types of impeller/vessels manufactured by Pierre Guerin (figure 1). In this study, the geometry is composed of a flat bottom vessel with four baffles, and a Pierre Guerin HTPG4 impeller (figure 1A). Vessel geometry and baffles were created using the 3D CAD modeler in Simcenter STAR-CCM+, and the impeller was extracted from a neutral CAD file format using the Simcenter STAR-CCM+ surface wrapping functionality, which was used to produce a closed volume from which an automated 3D unstructured polyhedral volume mesh was generated. One major advantage of the polyhedral meshing approach is the polyhedral cells have many neighbor cells (typically of the order of 10). This allows the transfer of variables across neighboring cells more efficiently. They can

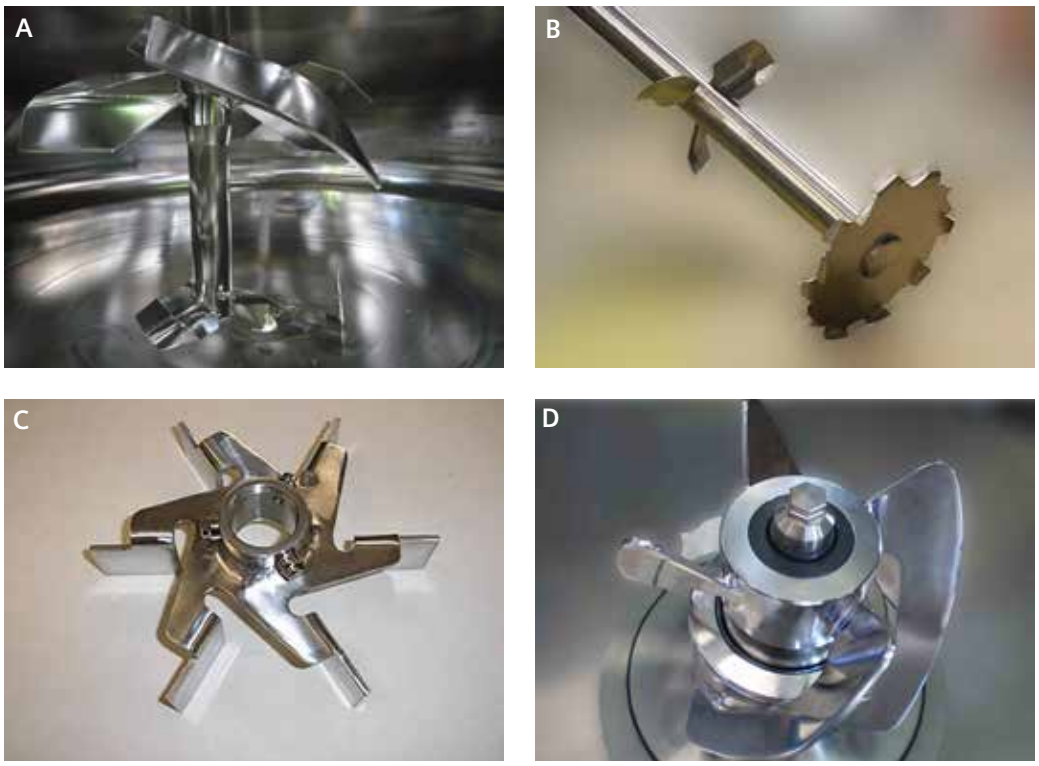


Figure 1: Different types of impellers manufactured by Pierre Guerin: (A) Low shear HTPG4 propeller for cell cultivation; (B) Heli Turbo Agitator HTA for powder dispersion; (C) Rushton turbines for aerobic fermentation; (D) Magnetic mixer PG-MAG for ancillary vessels.

better capture the intricate geometry at a much lower cell count than the tetrahedral mesh. The lower number of cells result in lower computational requirement.

Also, the global/local refinement capabilities of polyhedral mesh, along with the prism layer mesher at the boundaries, enabled engineers at Pierre Guerin to accurately capture the flow around the impellers, a key requirement for accurate power calculation. Figure 2 illustrates the computational mesh depicting fine mesh in the impeller region as well as boundary layers along the walls. The domain is divided with an interface between the outer stationary frame, which is attached to the vessel wall, and the central rotating part around the impeller. This resulted in a 400,000 cells in the domain.

Assumptions and boundary conditions

The process fluid for simulation was considered as a single phase liquid with constant density. The moving reference frame (MRF) method was used to simulate baffled stirred tank rotation [2]. The impeller motion was modeled using the rotor-stator approach. To model rotation of the shaft, the shaft part in the stator domain has a relative rotational speed in the opposite direction. The Reynolds Averaged Navier-Stokes (RANS) approach was used for turbulence modeling using the realizable k-ϵ two-layer model. It is not essential to know the flow detachment near the impeller blades. Therefore, there is no need to solve the viscous sublayer equation. But the boundary layer plays a role in the gradient generation; the buffer layer has to be solved. Use of this model has been verified with the wall y+ calculation, on the impeller and the shaft. Wall y+ was between 1 and 20. Because of the constant density flow and its incompressible character, the segregated flow solver is selected. In order to evaluate mixing, Simcenter STAR-CCM+ provides passive scalar approach. Passive scalars are user-defined variables of arbitrary value, assigned to fluid phases or individual particles with no

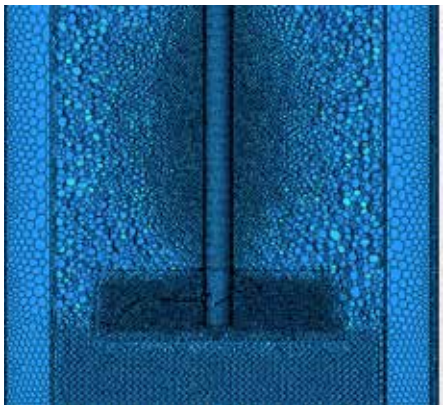


Figure 2: Polyhedral mesh in the computational fluid domain of the vessel and HTPG4 impeller using Simcenter STAR-CCM+.

appreciable mass or volume, and no effect on the physical properties of the simulation. It is also possible to define and inject more than one passive scalar in the domain. This capability is useful to trace a numerical dye injected in the flow stream as well as to analyze the mixing of two or more fluid streams that have the same properties. In this study, once the steady state solution was achieved, the flow solver was frozen, and the passive scalar transport equations were solved using implicit unsteady calculations and rigid body motion solver. The implicit unsteady solver equations have been solved using the second order upwind scheme.

Results

Convergence within the order of 10e-4 is achieved in about 17 minutes with a four-core parallelization of the computation. Figure 3 shows the numerical velocity vector field with an upward flow direction close to the walls/baffles, and a downward flow direction close to the impeller shaft. Numerical results of velocity field are available throughout the entire domain at any desired cross sections. Experimental measurement does not allow measurements in the full continuum of flow field data, and the engineering analysis is limited to the finite number of points at which measurements are taken. Access to the velocity and other fields in the domain gives valuable insights into the flow patterns and mixing behavior in the system.

Power and pumping number

In order to verify the accuracy of Simcenter STAR-CCM+ to predict the mixing performance, engineers at Pierre Guerin calculated characteristic numbers: power number, pumping number and a dimensionless mixing time. These numbers are unique to geometrical configurations as well as operating conditions. In order to calculate power draw unique to each type of impeller, the dimensionless number is defined as the power number (Np) that is calculated using the following formula:

$$N_p = \frac{\tau \, \omega \, g_c}{\rho \, N^3 \, D^5}$$

Where τ (N.m) is the resulting torque, ω (rad/s) is the impeller angular speed, N (RPM) is the impeller rotational speed, ρ (kg/m3) is the density, D (m) is the impeller diameter and gc is the gravitational constant.

Another dimensionless number that is used to calculate the flow or pumping rate unique to each geometric shape of mixing impeller is the pumping number (NQ). It can be calculated using the following formula:

$$N_Q = \frac{Q}{N \, D^3}$$

Where Q (m3/s) is the flow generated by the impeller, N (RPM) is the impeller rotational speed, and D (m) is the impeller diameter. These numbers are numerically calculated and compared with experimental results in table 1. As can be seen in this table, the results from Simcenter STAR-CCM+ are in remarkable agreement with those of the experiments as the percentage of difference for power number and pumping number are quite small (1.94 percent and 0.92 percent respectively).

In table 1, N.Tm is dimensionless mixing time, which is a product of the mixing time Tm with the impeller rotational speed (N).

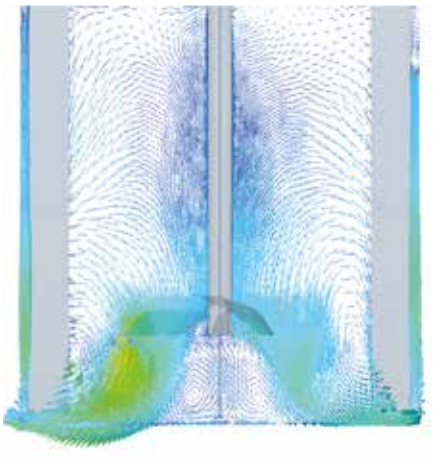


Figure 3: Velocity vectors and power number.

Mixing time

Mixing time is defined as the time required for achieving a certain level of homogeneity (in this case, 95 percent of ideal uniformity) of injected tracer in an operational stirred vessel [2]. It is used as one of the key parameters for evaluating the mixing performance. The general idea behind all of the experimental approaches is based on injecting a tracer into the mixture and then measuring its concentration over time, either visually or with several probes at different locations. Although these methods are spatially biased as they provide limited information about the entire domain, they have been widely used as the only available experimental tools. On the other hand, CFD can easily address this shortcoming of data by providing the flow and concentration field in a continuum space. This makes it possible to take into account the quality of mixing at every cell inside the numerical domain, and define a far more statistically accurate result for mixing time measurement.

In this regard, Simcenter STAR-CCM+ has a predefined equation for measuring volume uniformity throughout the entire domain. Mixed liquid has been tracked as a passive scalar, which is initially at rest at the bottom of the vessel (see figure 3, solution time 0.1 s). The passive scalar is like a numerical tracer mixed with water over time, and eventually the mixture achieves a

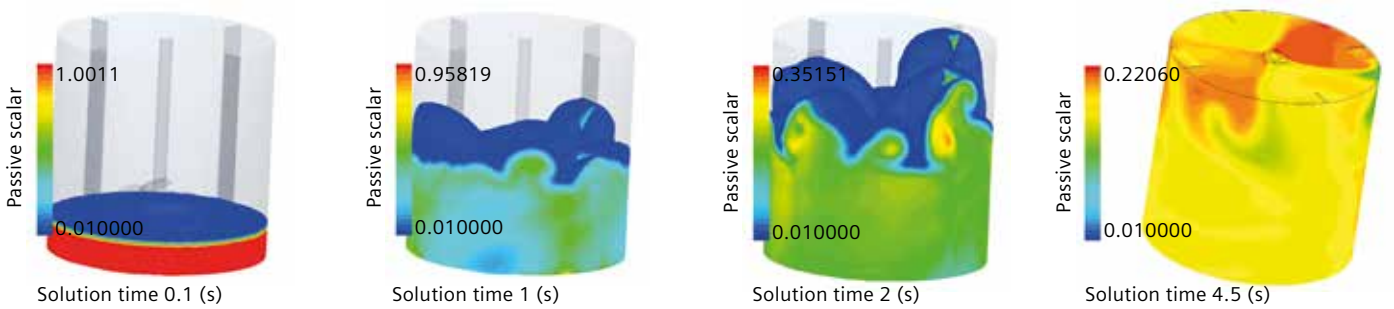


Figure 4: Time evolution of the passive scalar.

uniform concentration throughout the domain. Figure 3 illustrates the visual change in concentration of tracer over time. However, in order to quantify the uniformity, several points inside the domain are defined and the concentration of passive scalar tracer at these points are tracked over time. The results are shown in figure 5. For an ideal homogenous mixing, the mixing time is defined as the time required for achieving 100 percent uniformity at all of the tracer points (uniformity=1). In this study, achieving 95 percent uniformity for all the tracers was desired and has been used as the criteria for mixing time. The mixing time measurements are summarized in table 1.

Conclusion

Single phase simulation of a stirred tank equipped with an HTPG4 impeller has been modeled using different computational tools. CFD simulation results with Simcenter STAR-CCM+ provides accurate values as compared to experimental ones for the power number, the pumping number and the mixing time for a mechanically stirred tank. Compared to other tested software with comparable mesh element number, Simcenter STAR-CCM+ gives the fastest results while maintaining the same accuracy.

Also, the ease of use, hassle-free setup, and fast turnaround time for Simcenter STAR-CCM+ along with various types of postprocessing capabilities gives Pierre Guerin a remarkable advantage over its competitors in the market. This has given the company confidence in the use of Simcenter STAR-CCM+ for its future simulations.

	Experimental	Simcenter STAR-CCM+	Percent difference
N_P (power number)	0.67	0.657	1.94
NQ (pumping number)	0.65	0.644	0.92
N.Tm (dimensionless mixing time)	13	13.68	5

Table 1: Comparison between computational versus experimental results.

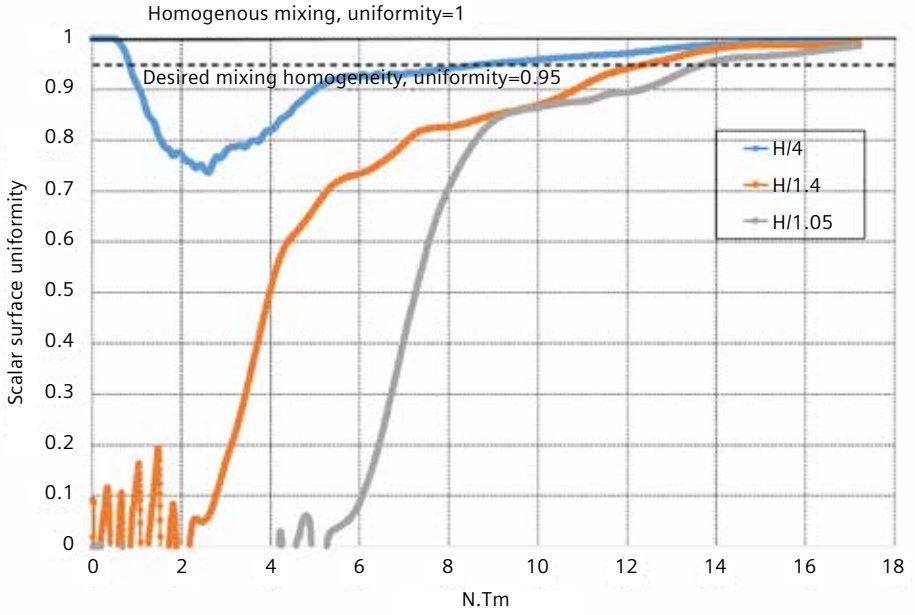


Figure 5: Time evolution of the passive scalar tracer concentration at different levels; dashed line on the graph indicates the desired mixing homogeneity (uniformity=0.95).

Computational analysis of FCCs

Introduction

Invented before World War II, the fluidized catalytic cracker (FCC) remains at the core of refining operations. Its role is critical in the profitability of refining operations since it cracks long chain hydrocarbons into more valuable products, such as gasoline.

Despite the age of the technology, FCCs remain the subject of significant study, both in design and operation. This article provides a brief overview of the role of computational fluid dynamics (CFD) and particle dynamics analysis, and two relevant case studies: modeling fluidization in an FCC riser, and the flow in a gas-solid cyclone separator. In both cases, simulation results are compared to theoretical or test data with excellent agreement achieved.

FCCs typically possess two components: a riser, reactor section and regenerator. In the riser section, hot liquid oil is injected, contacting hot catalyst particles. The resulting reaction causes the oil to be cracked and a the gas to expand, which drags the catalyst to the top of the reactor and into the regenerator where they pass through cyclonic separators. FCCs feature complex fluid and particle dynamics, heat and mass transfer. For simplicity, we will focus on two components: fluidization of solid catalyst particles, and flow in the cyclones. The fluidization analysis is typical of the type of study performed in the scale-up (from test bench to industrial) of a design, or when seeking to troubleshoot a maldistribution problem. The cyclone analysis can be used to improve separation efficiency, guarantee performance and minimize erosion damage.

Computational fluid dynamics

CFD is an analysis method widely used by engineers across disciplines, from oil and gas and chemical process to automotive and aerospace. Its use as a design tool was pioneered by the aerospace and automotive industries, where today it is routinely used to evaluate designs providing detailed insight, while reducing the time and cost associated with product development. It has been a key technology in improving the efficiency of vehicle engines, from modeling the complex fluid dynamics, spray, heat and mass transfer of an in-cylinder combustion engine, to the battery technologies in electric and hybrid electric vehicles.

In addition to solving fluid dynamics, heat and mass transfer, state-of-the-art CFD codes also include the ability to model particle motion. By solving both the fluid and particle dynamics we can begin to predict the complex behavior in an FCC.

One such method is discrete element method (DEM). Particles interact with each other and the surrounding geometry through surface contacts based on soft-particle formulation, where particles are allowed to develop an overlap. This approach enables detailed modeling of particle systems. It can then be coupled to a CFD simulation such that the particle motion is driven by particle-to-particle and particle-wall impacts and fluid forces.

Historically, DEM simulations would have been computationally prohibitive when modeling systems such as an FCC, since the computational cost of the analysis increases

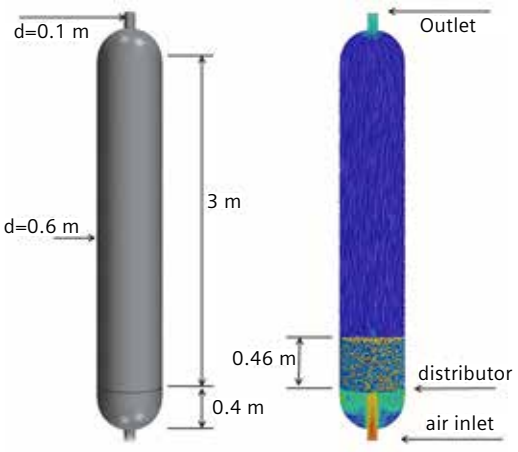


Figure 1: Geometry and boundary conditions for riser study.

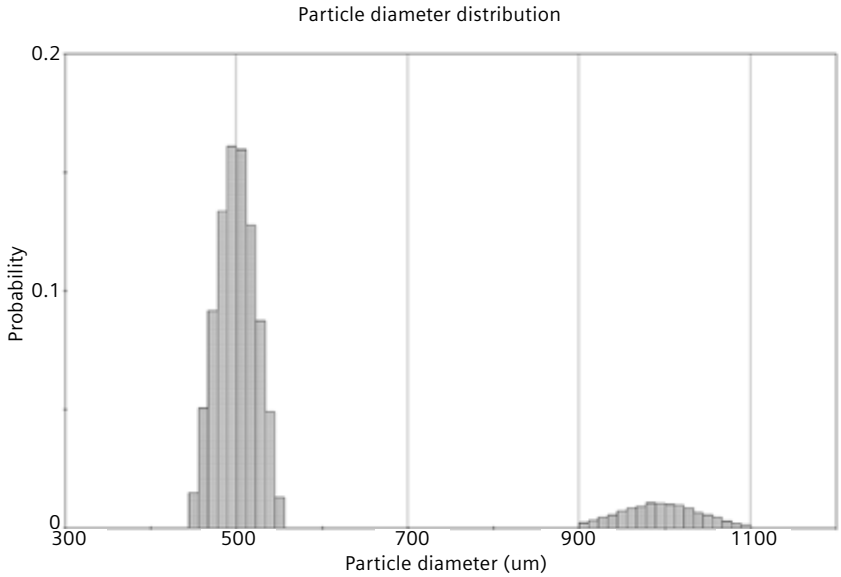


Figure 2: Size distribution of particles: fines with a distribution clustered around 500 microns and coarse particles around 1 mm.

with the number of particles modeled, and FCCs contain many billions of particles. Recent modeling advances introduced an approach called coarse graining. In coarse grain analysis, a large number of particles are represented by a single parcel. Fluid-particle interactions are calculated for a representative particle and applied to the entire parcel, while contact dynamics are calculated on the parcel scale. The method is then extendible to include the main physics of an FCC, including variable particle sizes, heat and mass transfer.[1]

Study 1: Modeling fluidization in an FCC riser

The system in this study is an industrial scale test facility (figure 1), 3 meters in height and 0.6 meters in diameter. The fluidized bed contains close to 1 billion solid particles, ranging from 500 micros to 1 millimeter in diameter.

The purpose of the study is to understand the fluidization behavior for different airflow rates, with comparison to Ergun prediction (a theory that predicts the fluidization behavior and resulting pressure drop). Such a study is typical of the type of analysis performed both in the design of FCCs; for example, to ensure successful scale-up from bench to industrial scale, to identify areas of maldistribution in the regenerator, or to understand the particle-to-particle forces, which can result in catalyst break-up.

The analysis process begins by defining the physical geometry of the riser, as shown in gray in figure 1. This is typically built in a parametric 3D CAD package. The parametric nature of the CAD model, and a tight link to the simulation package, enables engineers to quickly and easily explore the design space by varying the design and rerunning the analysis.

After the geometry is built, a computational mesh is generated. Various mesh or cell types can be used; this case a hexahedral mesh was used in the core volume, near-wall boundary layer and heat transfer effects were captured using what is known as a prism-layer mesh.

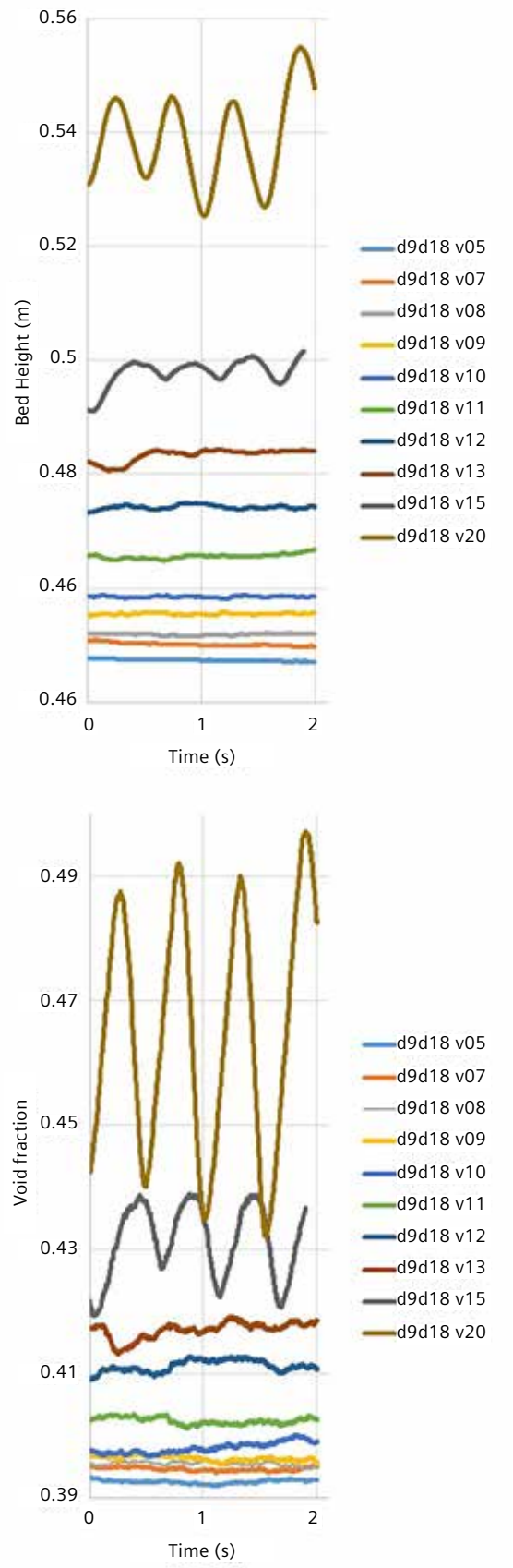


Figure 3: Time varying pressure drop and bed height for 10 superficial velocities.

That is a body fitted mesh, which efficiently resolves wall normal gradients by using prismatic cells. The hexahedral core transitions to the near wall mesh by trimming hexahedra to form polyhedral cells. This approach enables the use of hexahedra, which are desired because they provide greater accuracy with lower computational cost, even when working with complex geometries such as these.

After building the geometry and computational mesh, the physical properties of interest and boundary conditions are defined. In this case, incompressible air was used, varying the superficial velocity from 0.139 m/s to 1.139 m/s. One billion particles of varying sizes were modeled. The particles were divided into two broad sizes: fines and coarse particles. The fines were given a log normal distribution around 500 microns. The coarse particles had a mean diameter of 1 mm. The simulations were then run until a pseudo-steady state was reached, and variables such as pressure drop were averaged over the last two seconds of analysis time after ensuring that any start-up or initial condition effects had passed.[2]

As a validation step, the mean predicted pressure drop and void fraction of the bed for different superficial velocities is compared (see figure 5) with the Ergun prediction, an analytical theory for fluidized beds. Good agreement is achieved both in absolute values of the increasing pressure drop with increasing superficial velocity until fluidization occurs, and when the mean pressure drop stabilizes.

Study 2: Modeling the flow in a gas solid cyclone separator

In the second study, a detailed analysis is performed for a cyclone, as demonstrated during a presentation at the recent International Conference on Chemical and Process Engineering (ICHeaP) in Milan, Italy. Cyclones are used to separate the solid catalyst particles. The swirling of solid particles in the cyclone causes erosion damage. Poorly designed or performing cyclones cause a significant maintenance problem and cost. The ability to accurately predict the particle flow in the cyclone is used to troubleshoot existing designs, and to prevent such problems from occurring. In order to establish the accuracy of the simulation method, a standard cyclone test case was analyzed: Stairmand's cyclone. The benefit is that good experimental data is available for it.

Once again, a 3D CAD geometry was built, and the trimmed hexahedral mesh was used. The high swirl in cyclones means they are notoriously challenging devices to obtain accurate results for, and the industry practice was to use a structured, flow aligned hexahedral mesh along with an advanced turbulence model: the Reynolds Stress Model, or RSM. While RSM is still a requirement, this work demonstrates that accurate

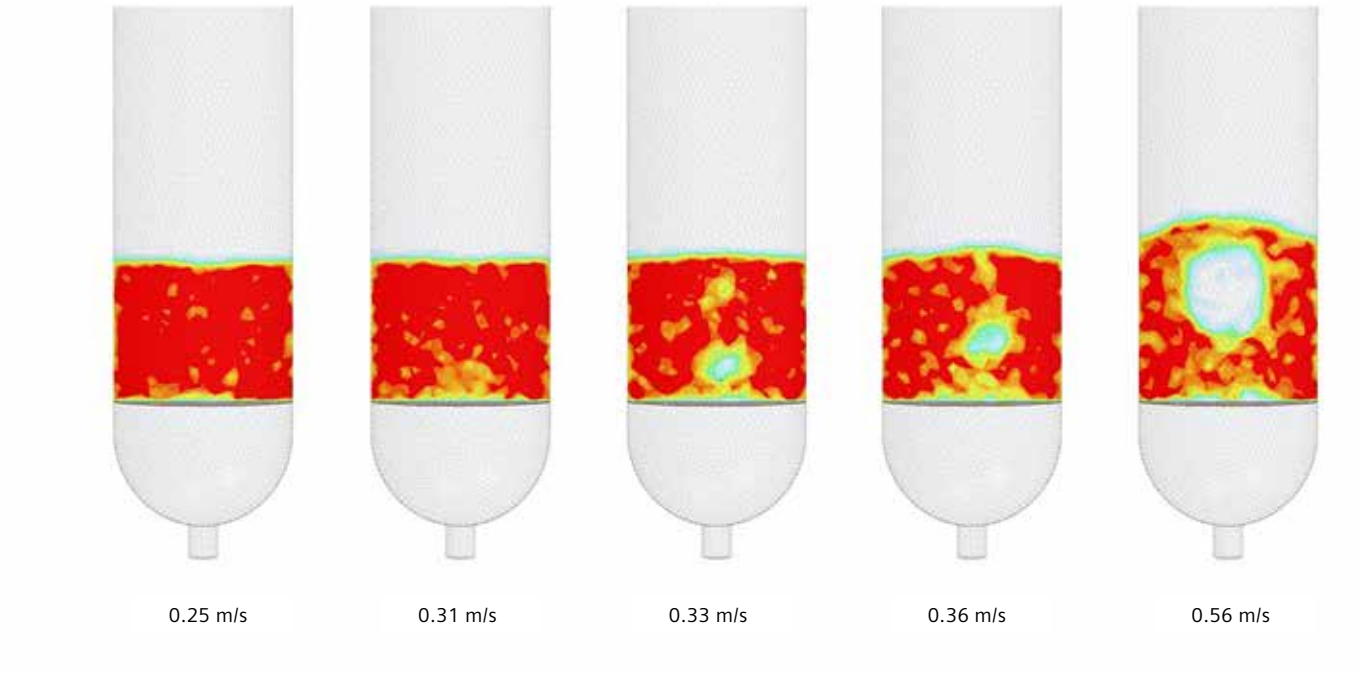


Figure 4: Size distribution of particles: fines with a distribution clustered around 500 microns and coarse particles around 1 mm.

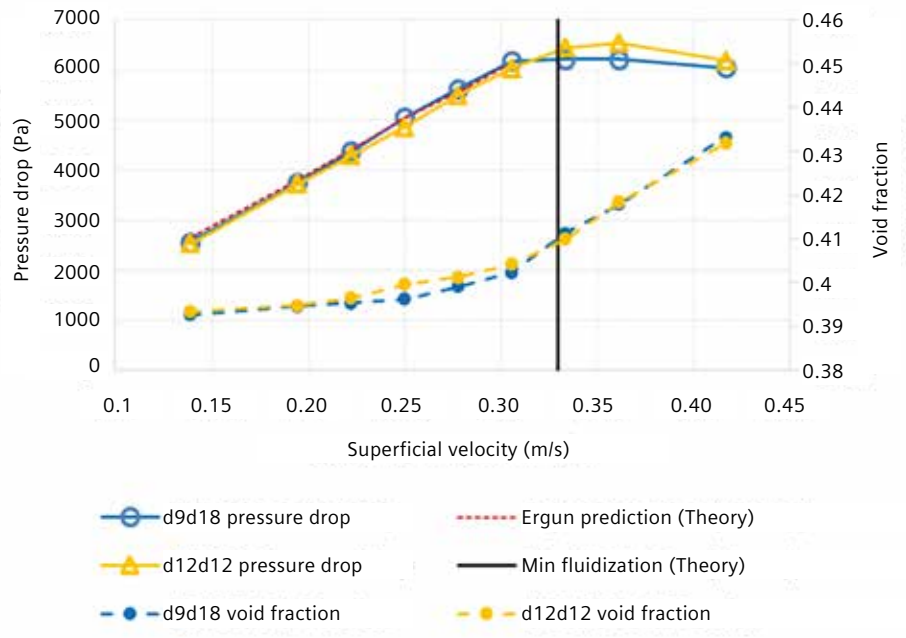


Figure 5: Mean pressure drop and void fraction against superficial velocity.

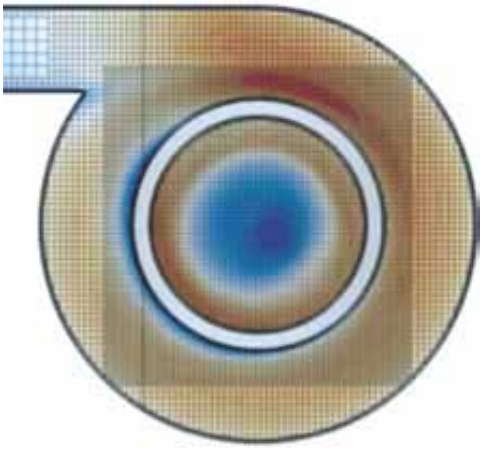


Figure 6: Cross sectional view of the cyclone geometry, mesh and contours of tangential velocity.

Figure 7: Streamlines showing the separation of heavy particles (lower outlet) and light particles via the central vortex.

results can be obtained while using an automatically generated hexahedral trimmed mesh, significantly reducing model setup times. A second outcome of this project was the incorporation of the simulation best practices into an automated workflow tool (a simulation assistant), that sits on top of the CFD packaged used (Simcenter STAR-CCM+).

In this case, the solid particles are sufficiently diluted so that the particle-to-particle

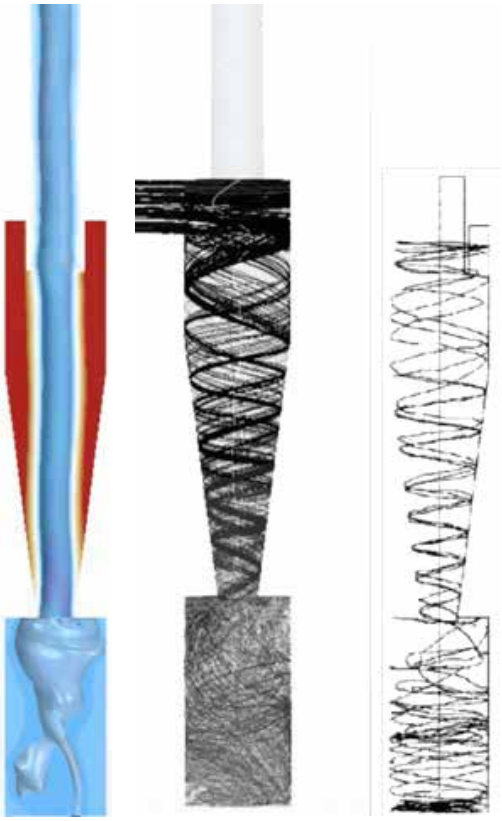


Figure 8: Snapshot of vorticity down the cyclone centerline, and particle trajectories – CFD (left) and experiment (middle and right).

interactions can be neglected and a traditional Lagrangian particle model can be used: Much the same as the DEM approach, this method predicts the path of the particle in the moving, particle reference frame, with the difference that particle-to-particle interactions are neglected, thereby reducing the computational effort. The particles can either have a one-way or two-way coupling to the background fluid: one-way being where the particle motion is driven by the flow, but the flow does not experience the presence of the particle. Figures 8, 9 and 10 demonstrate the simulation is able to accurately capture both the integral values of interest, such as pressure drop and separation efficiency, but also particle trajectories. The latter being the key input into an erosion analysis: erosion models correlate particle trajectory and velocity to wear or erosion rate.

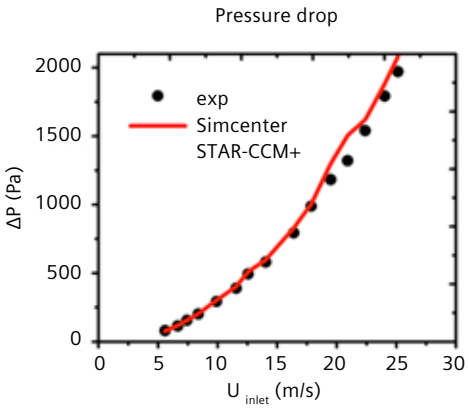


Figure 9: Average pressure drop across the cyclone versus inlet velocity: CFD and experiment.

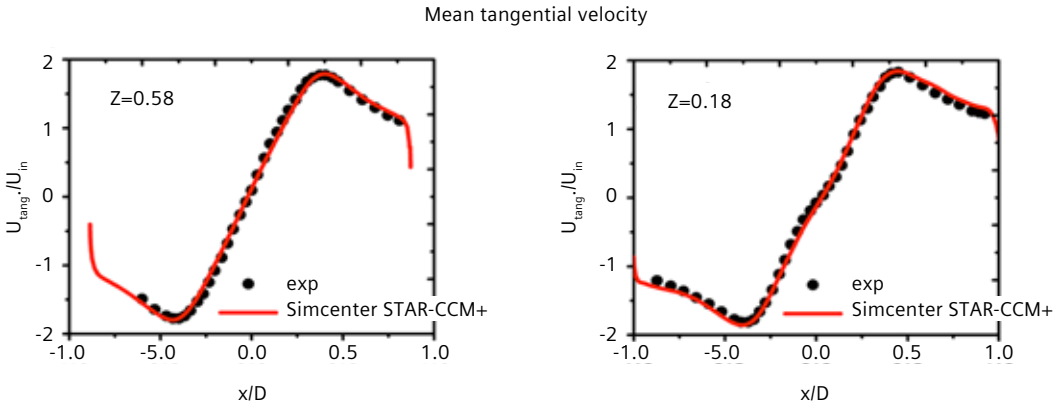


Figure 10: Average tangential velocity at two cross sections of the cyclone: CFD compared to experiment.

Conclusion

This article provides a brief overview of how state-of-the-art computational Fluid and particle dynamics tools can be used to design or troubleshoot FCCs, and FCC components, such as the riser or cyclone.

Specifically, it covers how advances in the DEM methodology, known as coarse graining, enables its application to systems with a large number (in excess of 1 billion) of particles with a reasonable computational effort, while yielding accurate results.

Secondly, accurate prediction of flow in cyclones can now be attained using high-quality, automated meshing techniques, such as the trimmed cell method described. When these are combined with workflow automation and best practice encapsulation tools, such as a simulation assistant, the effort involved in using CFD in the design or troubleshooting of devices, such as cyclone separators, is significantly reduced. Finally, hydrodynamics analysis of FCC requires hybrid approaches. Software such as Simcenter STAR-CCM+ offers the breadth of advancement lacking with long-existing traditional approaches. A DEM approach natively coupled with fluid flow is state-of-the-art.

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