Siemens Digital Industries Software

Simulation in the consumer products industry

Assessing the role of physics-based simulation in realizing a digital twin

Executive summary

This white paper describes the role that computational methods and simulation such as computational fluid dynamics (CFD), discrete element method (DEM), finite element analysis (FEA) and other system simulation methodologies must play in realizing a digital twin for digitalized enterprises in the consumer products industry (CPI). These technologies have an important role to play in validating and verifying the range, applicability and verity of a commonly used data-based and physics-based digital twin.[1] Several examples illustrate use cases and establish the importance of integrating various point simulation methods into a coherent digital thread to realize the full potential.

Ravindra Aglave, Glenn Longwell and Davide Picciotto,
Siemens Digital Industries Software

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Abstract

The consumer industry faces many challenges: A performance analysis of 34 of the world's top 50 consumer goods companies shows that 85 percent of those big companies had seen a decline in either revenues, profits or both. Only 15 percent managed to escape unscathed. Due to the health and environmental awareness of consumers, companies need to rapidly bring products to market to respond to their customer's needs. In the consumer products and cosmetics industries, consumers are now the primary influencers in the innovation process and ask for personalized products with unique experiences at no additional cost. This leads to the trend of smaller batch sizes to cater to diversified and to some degree, individualized needs.

The future of manufacturing will be largely consumer-centric and thus manufacturers must keep up with the newest trends while adapting their enterprises to become faster and more flexible while maintaining the highest levels of quality and security. More complex products meet new customer demands and once the product is designed virtually it is essential to understand and evaluate its manufacturability – this is enabled by advanced CFD simulations and more generically by computational methods and simulations. By bridging the gap between research and development (R&D) and manufacturing, manufacturing plans and processes can be executed seamlessly.

A holistic digital twin approach comprising product, production and performance and leveraging a solid collaboration platform enables a seamless transition between the virtual and the real world.

Smart process design uses digital representations of manufacturing unit operations to evaluate the performance of these steps. Using advanced engineering simulation to create a performance twin of the process, one can perform many trials for improved design to meet process requirements and optimize operations. This performance twin helps in tearing down the walls to the manufacturing process, resulting in an operation twin. Using automation, control simulation and virtual commissioning, the transformed recipes can be rapidly handed over to manufacturing sites.

The exploitation of data, computation and algorithms has exploded over the past decade. Bigger volumes of data with high-performance computing and advanced algorithms in machine learning (ML) and artificial intelligence (AI) are changing the way process engineering is performed. The combination of data and algorithms can result in models that can be used for predictive analytics.

The future will probably be a hybridization of both varieties of models. This paper investigates the role of physics-based models – such as those from CFD, DEM, FEA and system simulation – in the consumer products and cosmetics subsegment of the chemical and process industries.

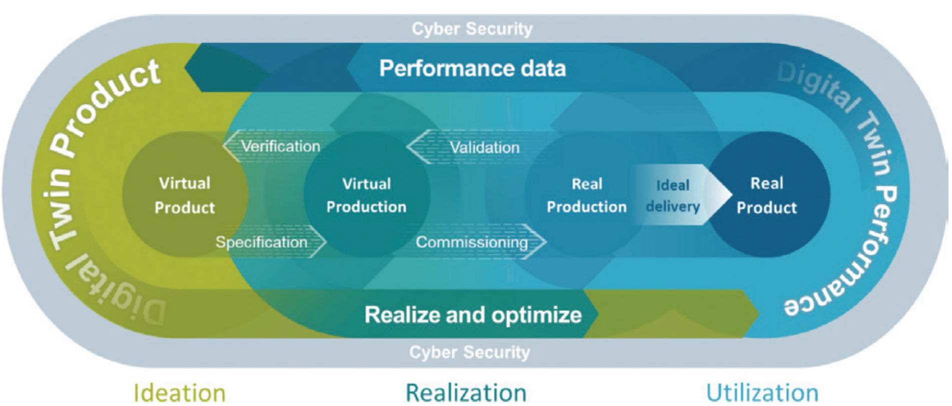

Figure 1: A schematic showing the Siemens vision of digitalization for the consumer products industry. Products are ideated and designed in the virtual world with the processes required to manufacture them, using simulations where needed to validate assumptions both on the product and production side and creating a digital thread.

Basic principles

The consumer products and cosmetics industries involve highly complex physico-chemical phenomena – multiphase flows, chemical reactions, heat and mass transfer. Flows are laminar as well as turbulent with Newtonian and highly viscous non-Newtonian fluids. Fluid-fluid interactions play a crucial role. Chemical reactions also occur due to electrothermal and electromagnetic forces. The processes become more complex as these interactions are scale-dependent. Consequently, equipment design has traditionally been based on the application of rules of thumb and experience. However, to remain competitive in the market and consistently produce quality products with higher yield, conversion and purity, the chemical industry is actively looking forward to using a comprehensive digital twin.

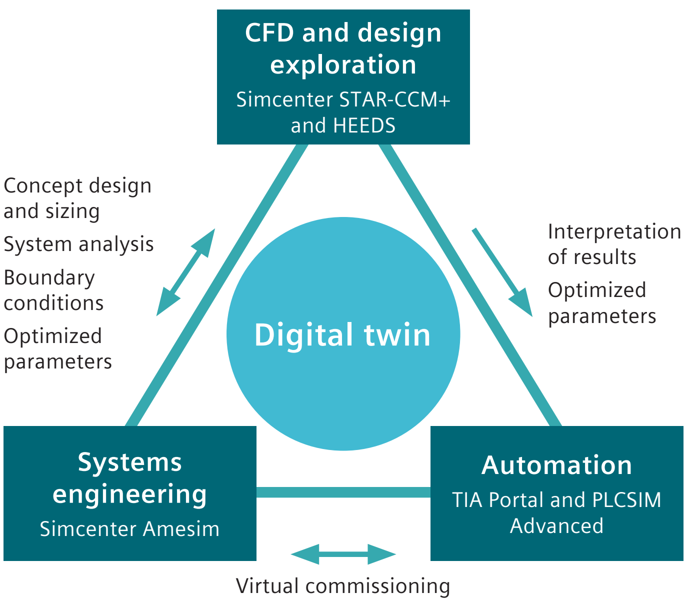

Figure 2: Essential elements of a performance digital twin for the process industries: simulation-based detailed engineering, system and process simulation and automation and control simulation.

Computational fluid dynamics has become an accepted technology for designing the chemical process equipment, unclogging performance bottlenecks, designing internals and evaluating innovative ideas. General purpose simulation platforms such as Siemens Digital Industries Software's Simcenter™ STAR-CCM+™ software solve partial differential equations originating from the most fundamental conservation laws of mass, momentum and energy. The conservation laws for a continuum can be expressed using an Eulerian or a Lagrangian approach as well as a combination of the two. In the Eulerian approach, a given volume represents a portion of space through which material can flow. In the Lagrangian approach, a given volume represents a portion of material in the fluid so an observer follows the material as it moves through space. Multiple physics – including fluid mechanics, solid mechanics, heat transfer, electromagnetism and chemical reactions – are also typically involved in a complex reactor.

Simcenter STAR-CCM+[2] has control volume methodology for both Lagrangian and Eulerian descriptions, whichever is most convenient for modeling a particular field of physics. For dispersed phases, Simcenter STAR-CCM+ offers a choice as it implements both Eulerian and Lagrangian descriptions to describe similar phenomena. Simcenter STAR-CCM+ has finite element method (FEM) for solid mechanics, electromagnetism and viscous flow applications.

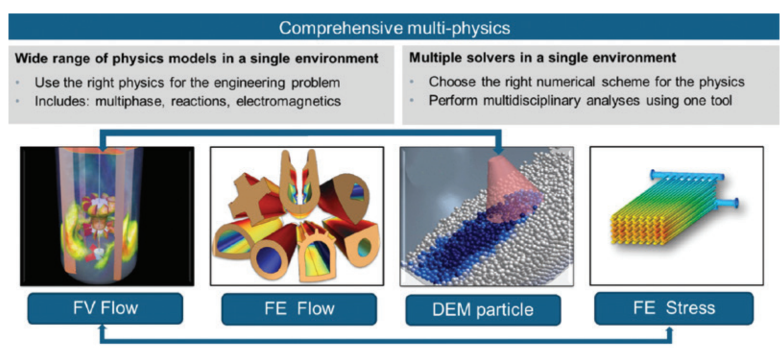

Figure 3: A key requirement for simulation is the ability to seamlessly combine, couple or interface various physics involved in the given process in a single platform such as Simcenter STAR-CCM+.

DEM is integrated in Simcenter STAR-CCM+. It is an engineering numerical method to simulate the motion of many interacting discrete objects that are typically solid particles. The distinct characteristic of DEM is interparticle contact forces are included in the equations of motion. These forces cannot be ignored for highly loaded flows (that is, flows with many interacting particles). Simcenter STAR-CCM+ uses a classical mechanics method to model DEM and is based on a soft-particle formulation in which particles are allowed to develop an overlap. The calculated contact force is proportional to the overlap as well as to the particle material and geometric properties.

Although Simcenter STAR-CCM+ offers models to represent complex physics, it provides robust polyhedral meshing technology in addition to standard tetrahedral and hexahedral meshers. Polyhedral meshes also contain approximately five times fewer cells than a tetrahedral mesh for a given starting surface, resulting in lower mesh counts and faster simulation. The new adaptive mesh refinement (AMR) feature lowers computational time for the same accuracy by dynamically refining the mesh where needed. The free-surface model-driven AMR intelligently refines cells to resolve the gas-liquid interface, reducing smearing. The overset-mesh model-driven AMR confirms that cell sizes at the interface are compatible. All of this is achieved without any user interaction.

Simcenter STAR-CCM+ also includes a finite element analysis solver for thermal and mechanical stress analysis and body deformation using mesh morphing methods. This makes it unique in providing a unified workflow.

Siemens has developed automatic controls for Simcenter STAR-CCM+, which dramatically improve the ease-of-use and robustness of the coupled solver. This delivers faster convergence-to-solution, giving users additional speed-up. All flow regimes, from incompressible through fully compressible, can be simulated straight out-of-the-box – no tuning necessary – with performance that rivals (and often exceeds) the best practices that used to take time and experience to develop.

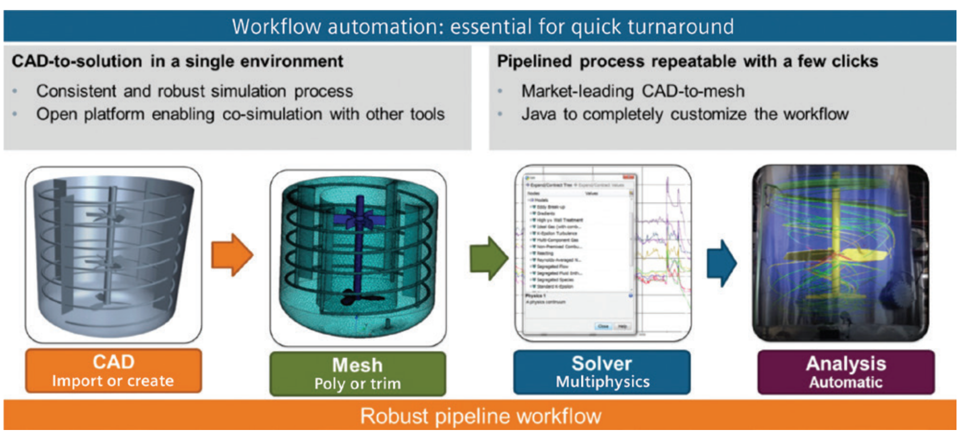

Figure 4: Evaluating the performance of a design or process requires exploration of the entire operating parameter space, mandating a robust and unified simulation workflow that can be effortlessly repeated.

Implementation

All the methods described above have their advantages and disadvantages in simulating equipment or (parts of) the process and should be carefully selected depending on the requirements. The huge benefit of applying CFD lies in the detailed information it yields about flow, mass, energy and species distribution. This enables detailed analysis and understanding of the interaction and dependency of the different variables, which cannot be achieved experimentally with a comparable accuracy and level of detail. Furthermore, simulations are inherently safe and cost-effective, especially when it comes to design or operating condition exploration, where changes can be applied instantaneously in the virtual world. These attributes have become even more important as 3D printing has emerged, eliminating many of the design constraints formerly imposed by traditional manufacturing processes. The following sections present a few examples of the use of Simcenter STAR-CCM+ to perform CFD simulations in combination with design space exploration in the consumer products and cosmetics industries.

Case studies

1. Process scale-up

One challenge in the food industry is taking innovative, flavorful creations from the lab and carrying out engineering designs to scale them to production level quickly while ensuring product safety, quality and uniformity. The engineering design of the process also needs to maximize the throughput along with minimizing energy and raw material usage.

Simulation can bring value to the scale-up process. Although the processing of many consumer goods involves complex multi-physics behavior, the rapid advances in computational power and techniques have brought many of these complex processes within reach to create high-fidelity predictive models. Typical examples are mixing, conveying, cooking, freezing, extruding and filling – wherever there are fluid flows, particle flows, heat transfer or (typically) a combination of all three.

Simulating the scale-up process can be viewed as a multi-step process. The product you want to scale up is first developed in relatively small quantities at laboratory scale. A simulation of that process is then performed to capture the physics and validate the model. From this you can gain a much greater understanding of the process and can then use simulation once again to design and analyze the pilot scale process. With the knowledge gained from the first model, at this stage you can begin to explore the design space to find innovative solutions. The pilot scale process is then produced. With validated results at two scales there is plenty of confidence in using simulation to design the full-scale process. In addition, the simulations provide deep insight into the process, including determining which variables are critical to scale-up. Of course, a large number of virtual experiments can be conducted in the full-scale process even when one does not have the time or resources to perform these trial-and-error experiments on the actual equipment.

In the food and beverage industry, safety and sterilization are of utmost importance. It's also one area where simulation can provide the kind of guidance required to scale up the process – a sterilization process may work very well on a small scale but may face difficulties at production scale. This is primarily because various physical behaviors such as heat transfer, mixing and suspension scale differently with the size of equipment and throughput. Time-to-market and energy usage to sterilize products can affect the profitability of a product. Often, only a limited number of experiments with limited numbers of temperature probes are feasible. And in most cases many critical variables cannot be measured inside a sealed food container without affecting the process itself. Simulation provides a virtual temperature probe everywhere inside the domain of interest.

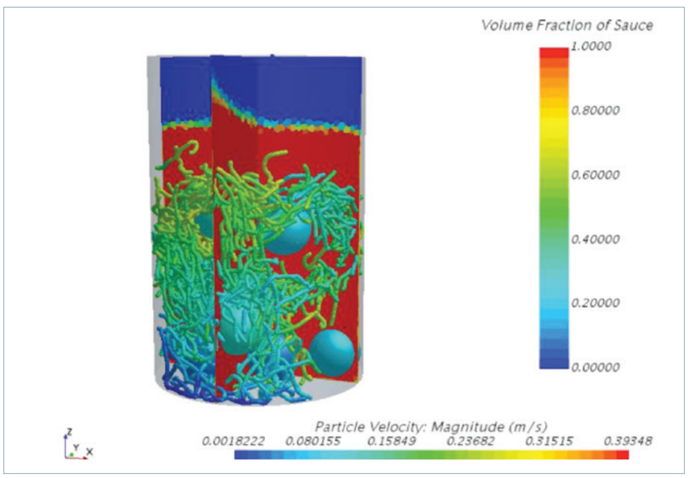

Figure 5. Contour plots of volume fraction of tomato sauce and velocity of solid particles (meatballs and spaghetti) in a can.

ConAgra Brands, Inc.[3] performed simulations of a rotary retort using Simcenter STAR-CCM+ to gain insight into the sterilization process. The system under consideration consisted of both liquids and multiple solids (shapes) with varying properties. The goal was to ascertain that each of the solids had reached the necessary temperature. Simulation can provide a level of insight that is difficult or impossible to obtain with experimentation. This application illustrates the need for a software solution that can easily handle both fluids and solids within the same simulation environment, like Simcenter STAR-CCM+. Simulation helped ConAgra speed the scale-up process for a spaghetti with meat balls in a tomato sauce, while increasing process efficiency and minimizing quality losses. Sohan Birla, principal research engineer at ConAgra, says, "The Simcenter STAR-CCM+ DEM functionality helped us to simulate very complex heat transfer in the can filled up with food particulates. The model provided a deep look inside the can undergoing complex rotating and translatory motion in the retort."

Similar research work was done by Jafari[4] in spray cooling of hot tomato juice cans. Simulation was used to understand cooling behavior as a function of the rotation rate of cans and spray characteristics. Simulation provided insight into the heat transfer and fluid dynamics of what was happening inside the can. From this knowledge the simulation can now be used to determine operating conditions to optimize for throughput, energy and water efficiencies during the scale-up process.

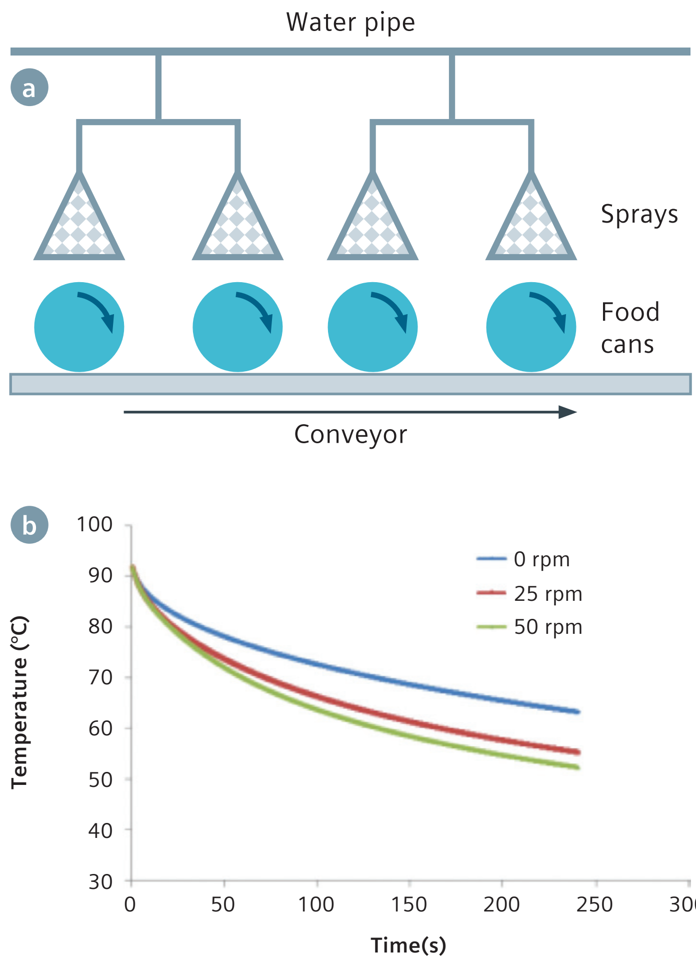

Figure 6: (a) The spray cooling system showing rotating cans on a conveyor. (b) Effect of rotation rate on cooling of cans calculated using CFD simulation of spray and heat transfer with Simcenter STAR-CCM+.

2. Packaging design

The consumer's experience using a product determines if the product will be liked and adopted. It has a critical impact on the commercial success of the product. Such user experience can range from the bottle squeeze to the dose of a cosmetic product like shampoo or a food product like ketchup.

- **Drip-free laundry detergent bottle**
  Unilever's goal was to design laundry detergent bottles that can pour without spilling or dripping. Such a design needs to account for the flow of a Non-Newtonian liquid through the nozzle of the bottle. The nozzle design needs to be large enough to have a comfortable flow but still prevent spilling detergent. Unilever had primarily relied on experimental methods by creating prototypes of the bottles and testing them for drip analysis. With the help of Simcenter STAR-CCM+ running on a supercomputer, Unilever was able to shift to a completely virtual process to test the prototypes.

Figure 7: Simcenter STAR-CCM+ simulation showing the pouring process from a typical laundry detergent pack with a close-up of the nozzle design.

The development time was reduced from 20 weeks to two weeks for one project alone.[5] Furthermore, there was 50 percent less overall time needed to launch the product into the market and 55 percent reduction in the cost required to develop the packaging.

- **Dosing from a ketchup bottle**
  Dosing rate can be calculated using fluid flow and structural simulations that can account for the structural behavior of the packaging as well as the non-Newtonian fluid behavior of the ketchup. Such a framework can be utilized to create a rapid prototyping workflow for designing new packaging for product launches.

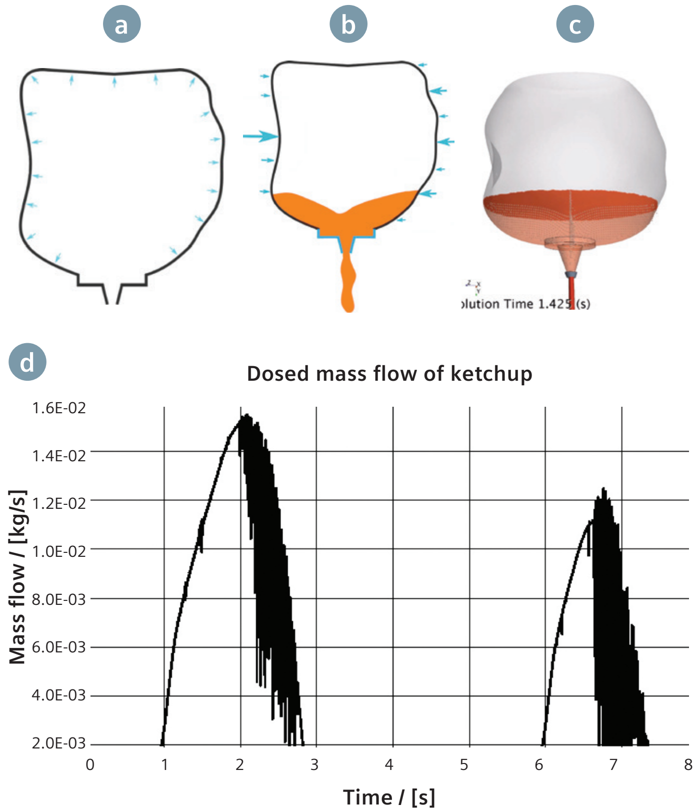

Figure 8: (a) Schematic of a ketchup bottle with simulated fingers.
(b) Schematic showing flow of liquid due to squeezing of the bottle.
(c) CFD simulation showing dispensing of ketchup. (d) Dosage of ketchup.

- **Making stronger and lighter bottles**
  Design of a glass bottle is another example in which the user needs to account for the complex material behavior of glass, the press and blow process of bottle formation and thermal simulation of the cooling process. Bottero has successfully used simulation to design bottles that are lighter without loss of strength.[6]

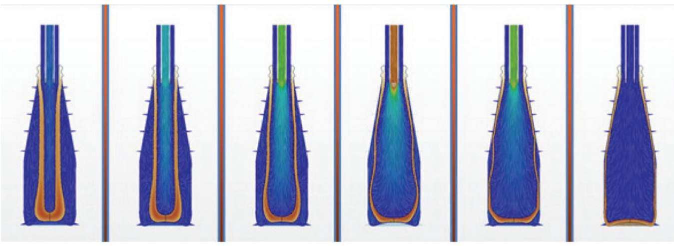

Figure 9: Snapshots of the press and blow process simulation with time (starting from the left). Bottero uses simulation to design bottles that are lighter (less mass) but stronger for the purposes for which they are intended. Image courtesy of Bottero.

3. Virtual commissioning of bottle-filling machines

Simcenter Amesim™ software includes ready-to-use multi-physics libraries combined with application and industry-oriented solutions that are supported by powerful platform capabilities to let you rapidly create models and accurately perform analysis of complex systems. It is an open environment that can be integrated into enterprise processes for design and optimization. Ronchi Mario, a bottle filling machine manufacturer, used Simcenter Amesim to investigate design choices that would maintain pressure in the filling lines. The entire system simulated using Simcenter Amesim consisted of a tank, pump, many meters of piping through which the fluid was pumped and several dosing valves that injected the fluid inside the containers that needed to be filled. Performing simulations allows you to commission the machine virtually and get it right the first time it is operated, saving a lot of time, sometimes several weeks. Due to the highly accurate simulation using Simcenter Amesim, Ronchi Mario has reduced the number of prototypes it typically produces by up to 20 percent per project. Simulation enables the team to predict machine behavior and determine the best design before prototype production.

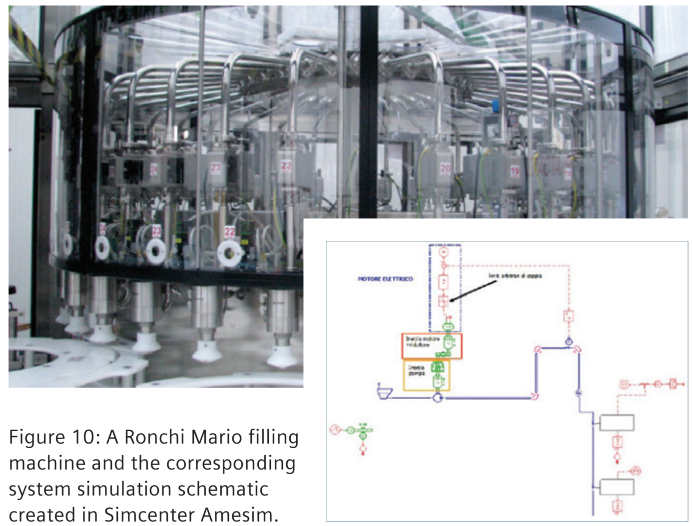

Figure 10: A Ronchi Mario filling machine and the corresponding system simulation schematic created in Simcenter Amesim.

Siemens anticipates integrating results from high-fidelity CFD simulation solutions like Simcenter STAR-CCM+ into Simcenter Amesim system simulations. For example, a full 3D analysis of valves can be carried out with CFD simulation, with Simcenter Amesim providing the boundary condition evaluation and 3D CFD providing detailed behavior insights. This kind of co-simulation combines the complementary strengths of both types of simulations to deliver the best analysis of entire systems.

4. Spray dryer: coupling CFD and process simulation

Spray dryers are widely used to produce powder out of a slurry feed by using a hot gas stream. But designing and optimizing the dryer chamber strongly depends on the process and the processed materials. Typically, it cannot be done without the upstream and downstream components, namely separation equipment like cyclones or filters as shown in figure 11. The design is typically performed with a process simulation tool like gPROMS, where each piece of equipment is represented by a simplified model, often a 0D or 1D model. This makes the process simulation extremely fast but neglects any inhomogeneity, which can affect the predicted performance significantly, especially in the spray dryer unit where large velocity and temperature differences may occur. These differences can be quantified by a CFD simulation, but typically the runtime of a CFD simulation is orders of magnitude longer and cannot be combined directly with a flow-sheet simulation. A hybrid multi-zonal coupling approach can overcome this limitation: a converged CFD simulation is split into a few zones, each with roughly constant properties. Averaged flow properties and fluxes from these zones are passed to a reactor network on the process simulation side. With this approach, the inhomogeneities are made available to the process simulation and significantly higher accuracy can be achieved.

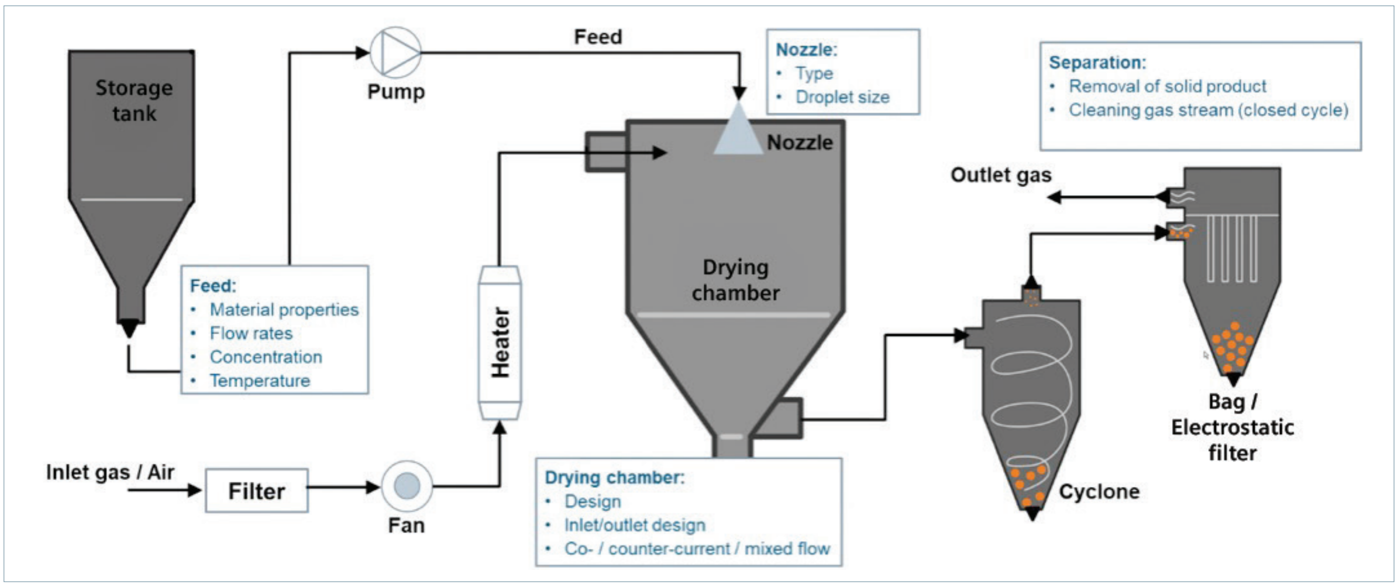

Figure 11: Flow sheet of a generic spray drying process. To optimize the drying chamber the upstream and downstream equipment need to be considered.

Directions in simulation for the consumer products and cosmetics industry

Currently, various simulation elements are used as point solutions, which are disconnected from each other. Digital threads that run through a digital twin or point solutions require interfacing between each of the point solutions. This work is well underway at Siemens.

As summarized in the article *Simulation in the lifecycle of a process plant*,[8] "In the future, simulations will be systematically used and will be an integral part of the normal engineering and operating processes over the entire lifecycle of process plants. The basis for the engineering and operation of a plant will be a virtual depiction of the plant. Decisions will be evaluated and made based on the virtual plant. New plants will first be planned and developed virtually, and even in existing plants no changes will be made before a preceding check in the virtual plant. Once developed, models will be re-used and refined over the course of the lifecycle. This will be supported by available exchange and co-simulation standards. The configuration of the simulation models is done modularly to allow re-use and an efficient layout. Simulation models (modules) can be connected to each other in the sense of plug-and-simulate.

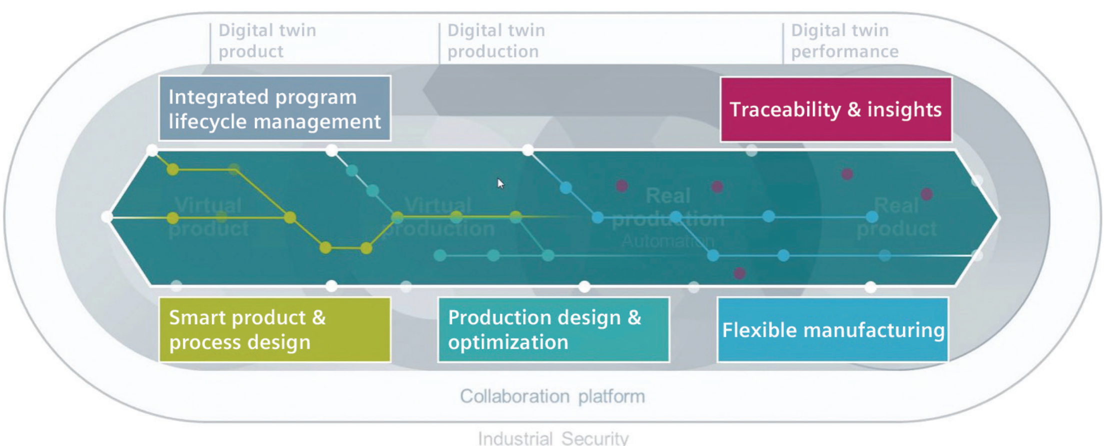

Figure 12: As an integrated ecosystem of digital technologies, few critical industry-specific digital threads work together to tackle the challenge of integrating the real and virtual worlds in ways that promise to revolutionize how products are ideated, designed, made and then delivered.

Conclusion

The consumer product industries involve a wide variety of flow complexities ranging from single phase gas and liquid flows to multiphase flows like gas-liquid, gas-solid, liquid-solid and gas-liquid-solid flows. The processes generally involve fluid-solid interactions, particle size distributions, heat transfer, mass transfer and combustion. CPI is making a strong shift from traditional rule-of-thumb-based approaches controlled by design experts to simulation-based approaches. Even the historically conservative pharmaceutical industry is adopting engineering simulation-based platforms to evaluate equipment designs and complete flow sheets to achieve desired performance and reduce their dependence on experimental evidence. Industry is recognizing the importance of the digital twin in all three of its forms – a twin for product, production plant and the model-based digital twin of the performance of either the product or the production process. Simcenter STAR-CCM+, Simcenter Amesim, Simcenter 3D and gPROMS are some of the leading computational tools that offer modeling alternatives to realistically represent the complex physics involving single phase and multiphase flows with chemical reactions, gas, liquid, solid combustion, heavily loaded particulate flows coupled with electrochemistry, thermoelectric and electromagnetic processes.

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Siemens Digital Industries Software

Headquarters
Granite Park One
5800 Granite Parkway
Suite 600
Plano, TX 75024
USA
+1 972 987 3000

Americas
Granite Park One
5800 Granite Parkway
Suite 600
Plano, TX 75024
USA
+1 314 264 8499

Europe
Stephenson House
Sir William Siemens Square
Frimley, Camberley
Surrey, GU16 8QD
+44 (0) 1276 413200

Asia-Pacific
Unit 901-902, 9/F
Tower B, Manulife Financial Centre
223-231 Wai Yip Street, Kwun Tong
Kowloon, Hong Kong
+852 2230 3333

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Siemens Digital Industries Software is driving transformation to enable a digital enterprise where engineering, manufacturing and electronics design meet tomorrow. Xcelerator, the comprehensive and integrated portfolio of software and services from Siemens Digital Industries Software, helps companies of all sizes create and leverage a comprehensive digital twin that provides organizations with new insights, opportunities and levels of automation to drive innovation. For more information on Siemens Digital Industries Software products and services, visit siemens.com/software or follow us on LinkedIn, Twitter, Facebook and Instagram. Siemens Digital Industries Software – Where today meets tomorrow.

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