M-STAR

How AbbVie Built Accelerated Digital Twins to Understand Miscible Fluid Blending

Predicting real-time fluid mechanics within a physical mixing tank with a fidelity that rivals experimental data.

Pharmaceutical companies like AbbVie face unique mixing challenges in the manufacturing process, causing significant processing and scale-up issues. Where literature correlations, experiments and numerical modeling fall short, CFD software excels.

With M-Star CFD, AbbVie built accelerated digital twins of a physical mixing tank to predict real-time fluid mechanics with a fidelity that rivals experimental data.

The following case study follows findings from research featured in AAPS PharmSciTech, 2021.

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About AbbVie

AbbVie is an American research-based biopharmaceutical company headquartered in Lake Bluff, IL, that focuses on discovering and delivering transformational medicines and products in several key therapeutic areas including immunology, oncology, neuroscience, eye care, virology and women's health.

Problem

In the biopharmaceutical manufacturing process, mixing stratified miscible fluids with widely different material properties – namely densities and viscosities – is a common step.

However, the differences between fluid densities and viscosities can lead to order-of-magnitude increases in blend time relative to the blending of single fluid systems. Plus, the mixing performance in two-fluid systems can be strongly dependent on the position of the impeller relative to the fluid interface.

Due to the complexities of the fluids involved and engineering design limitations, manufacturers struggle to scale-up production.

The problem extends further when you consider three common solutions and their limitations:

Traditional Solution Limitations		
Literature Correlations	**Numerical Modeling**	**Experiments**
Few literature correlations exist for two-fluid systems with large differences in density and viscosity.	The transport physics are three-dimensional, spatially varying and evolve in time, limiting the applicability of RANS equation-based turbulence models and other time-averaged fluid modeling approaches.	Experimental approaches are limited by equipment access, material expenses and specialized labor costs.

Solution: A Hybrid Approach

To solve for the limitations of traditional approaches, AbbVie turned to a hybrid approach.

With M-Star CFD, AbbVie combined lattice-Boltzmann transport algorithms with GPU-based hardware to build accelerated digital twins of a physical mixing tank. This essentially hybridizes the three approaches by developing a digital replica that can run real-time numerical experiments based on the appropriate mathematical models.

Note: Developing a digital twin does not eliminate the need for experiment

- Relevant fluid properties must be measured and supplied to the twin.
- Appropriate experimental blend-time and power number data is crucial for validating output.
- Efforts must be made to ensure that the results are time-step and grid-spacing converged at the operating conditions of interest.

Results

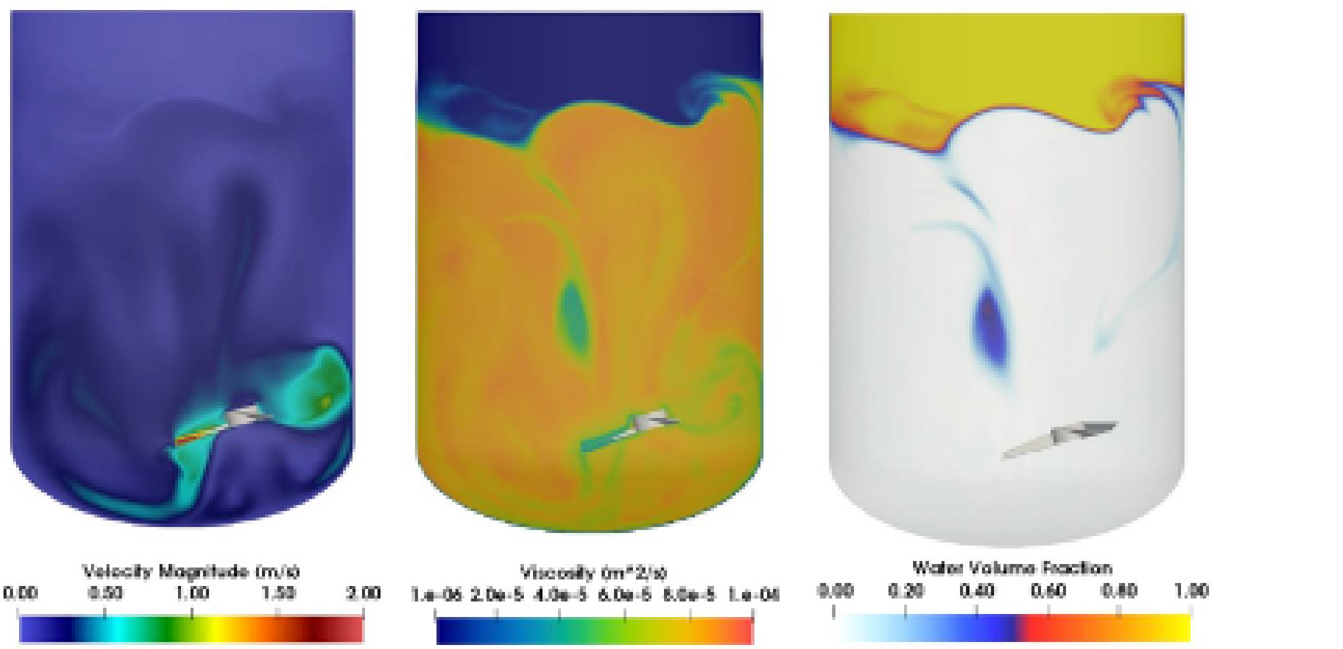
The method allowed AbbVie to simulate minutes/hours of fluid mechanics within just hours/days of computer wall time. Once developed, digital twins can be used to generate transient processing insights with a fidelity that rivals experimental measurement but at a much lower cost.

The Value of a Digital Twin

Output Reproducibility: Predictions from a digital twin should be indistinguishable from measurements on physical equipment.

Time & Resource Scalability: The twin should compare favorably against experiments in terms of time and resources required to obtain comparable information.

Process Applicability: Predictions from multiple in silico experiments using the digital twin should be able to generate process design correlations.



A snapshot of the system velocity, viscosity and water volume fraction during the agitation process for the 494 RPM operating condition. This snapshot was generated after 82 impeller turns, a time observed to be sufficient to realize steady-state flow conditions across the bulk of the vessel. The power number of the impeller calculated from the predicted power draw at steady state is 0.35. This power number prediction is consistent with measured data at these operating conditions.

About M-Star CFD

M-Star Simulations, LLC, is a software company focused on the development of computational tools for modeling momentum, energy and mass transport within engineering and biological systems. By pairing modern algorithms with GPU architectures, this software enables users to quickly perform calculations with predictive fidelity that rivals physical experiment. These outcomes are achieved using a simple graphical interface that requires minimal user specification and setup times.

Founded in Maryland in 2014, M-Star Simulations has grown to include commercial, government and academic users across North America, South America, Europe and Asia.

Struggling to scale-up production due to complex fluid physics and engineering design limitations? M-Star can help.

Contact us for a demo or free trial.

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