Qualification of Mixing Operations Using Computational Fluid Dynamics

When scaling up a mixing operation there are a number of process parameters that can drastically alter the quality or yield of the desired product. Factors such as shear rate, vorticity and bulk movement are all critical design considerations for large scale mixing (Paul, Obeng, and Kresta, 2004). Often it is difficult to directly compare these factors between varying production scales due to the empirical nature of current mixing characterization methods. By combining Computational Fluid Dynamics (CFD) modeling with conventional methods it is possible to develop a strong understanding of a given mixing process, enabling goodengineering design practices.

CFD METHODOLOGY

A CFD mixing study consists of three primary phases: pre-processing, solving, and post-processing (Chung, 2002). During pre-processing a mesh is generated for the physical system, often using a 3D CAD model or drawing. Pre-processing is also when the boundary and initial conditions are determined. These factors greatly affect the quality of a CFD study; great care is taken to ensure that these constraints are set appropriately.

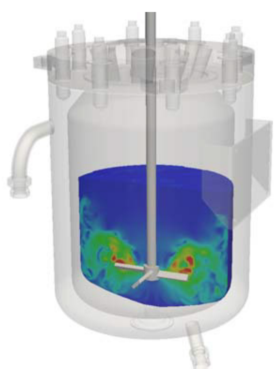

Figure 1. CFD Simulation: Visual of fluid shear stress on 2L lab reactor at 300RPM using P4 type impeller

Furthermore, the thermophysical properties of the materials are identified during this phase. These include: viscosity, density, heat capacity and surface tension. Next the solver is setup by the CFD engineer to best accomplish the goals of the study. This is accomplished with the use of proprietary packages (ANSYS, SolidWorks) or inhouse solutions. Lastly, during post-processing the CFD engineer works closely with the client or design engineer to guarantee that the relevant data is obtained in a presentable and functional manner.

APPLICATION TO SCALE-UP DESIGN

CFD studies are best used alongside conventional methods for mixing design. CFD analysis can be crucial when performing scale-up design for novel materials as industry best practices lag behind development. The role of CFD in mixing design can be broken down as follows,

Process design: reactor temperature, head pressure, RPM, etc.

Equipment design: impeller type, reactor geometry, sparger placement, etc.

CFD studies can be used to validate operating conditions (RPM - bulk mixing), troubleshoot unknown effects (temperature profile - degree of reaction), and identify proper equipment selection (impeller type – shear). When used appropriately CFD studies can be applied to optimize mixing conditions and equipment, leading to improved process safety and decreasing capital and operating costs. SolidWorks and OpenFoam are software packages that enable accurate CFD simulations and are used extensively by the engineering team at XRCC. CFD studies are employed to develop scalable processes and operations that ensure comprehensive engineering design and client satisfaction.

ABOUT

The Xerox Research Centre of Canada is Canada's leading materials research centre, home to a world-class team of scientists focused on taking materials from concept through to market in a highly competitive technology environment. Our core expertise is the design, synthesis, formulation, and scale-up of novel materials. We specialize in Process Engineering, Materials Supply, Technology Transfer, Synthesis, Formulation, Polymers, Composites, Coatings, Nanomaterials and Electronic Materials.

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References

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Paul, E. L., Obeng, V. A., & Kresta, S. M. (2004). Handbook of Industrial Mixing. John Wilely & Sons Inc.

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