Simulation Based Optimization of Stirred Tank Reactors

Extended Abstract for the 2014 Annual AIChE Conference

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May 12, 2014

The design of a stirred tank reactor is a multi-input and multi-output problem. Design parameters may include geometric variables (impeller geometry, baffle geometry etc.) and operating conditions (impeller RPM, fill level etc.). Some common design objectives are minimizing mixing time, maximizing mixing quality, achieving a specific scale of agitation etc. Additionally, various constraints can be imposed on the performance of a reactor, such as avoiding overflow, avoiding mixing 'dead zones', imposing a maximum shear stress etc. Designing to these multiple objectives and constraints by modifying a large number of design parameters is a challenging task since the relationships of these multiple inputs and outputs can be highly non-linear. Therefore, the design of stirred tank reactors has traditionally been a very repetitive and time-consuming task. This is the primary motivation for developing a design methodology that is both autonomous, and efficient in targeting specific reactor performance.

Optimization algorithms lend themselves well to solve such multi-input, multi-output problems. An optimization algorithm iteratively runs evaluations and understands the sensitivities between all inputs and combination of inputs to all outputs. The algorithm successively guesses a better design until a converged design is reached that optimizes all the required objectives while satisfying all constraints. This study details the implementation of this optimization methodology to design optimal stirred tank reactors for various design objectives and constraints.

The use of an optimization algorithm for design studies requires two components: an analysis tool and an optimization algorithm. The optimization algorithm uses the analysis tool to generate the relationship between a set of inputs and outputs. Figure 1 graphically represents the implementation of the analysis tool within the optimization process.

The analysis tool for this study is STAR-CCM+, which is a multi-physics simulation platform provided by CD-adapco. The reactor is analyzed using a Computational Fluid Dynamics (CFD) approach. The use of STAR-CCM+ for mixing tank performance prediction has been validated by the work of Maaß et al [1]. The stirred tank reactor geometry was created to be fully parametric with 22 different geometric parameters. These parameters deal with overall tank geometry, impeller

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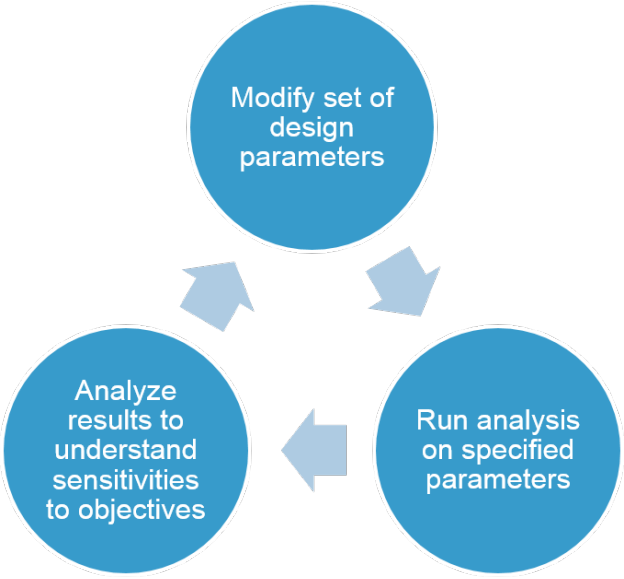


Figure 1: Schematic of optimization process

geometry, impeller blade geometry and baffle geometry. A polyhedral computational mesh with prism layers on all walls was used. Depending on the design objectives, two types of simulations were run, steady and transient. The steady state (time averaged) cases use a Moving Reference Frame (MRF) approach, which solves the fluid equations in a rotating reference frame around the impeller. The transient (time accurate) cases use a Rigid Body Motion (RBM) approach, which physically rotates computational mesh for the spinning region. For all of the simulations, a passive scalar approach is taken to track the quantity of mixing throughout the reactor.

The highly efficient SHERPA algorithm was used to drive the optimization study [2]. The acronym SHERPA stands for Simultaneous Hybrid Exploration that is Robust, Progressive and Adaptive. During a single search, SHERPA uses multiple search methods simultaneously (not sequentially). This approach takes advantage of the best attributes of each method and reduces a method's participation in the search if/when it is determined to be ineffective. From a usability standpoint, the SHERPA algorithm is extremely easy to use since it only has a single tuning parameter (total number of evaluations), as compared to traditional algorithms which require a high level of expertise to apply.

The authors have previously used the same methodology and tools to generate some preliminary results [3]. This study will extend the previous work by running optimization cases with more rigid requirements and constraints. This will serve to highlight the applicability of this method for cases in which manual designer intuition can be extremely difficult. Finally, some data will be reduced about the trends observed during the optimization process which will help gain further insight into the behavior of the generic mixing tank reactor system.

References

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