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

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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 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 aspect of the design process including mechanical, electrical, and chemical components. From mechanical perspective the design parameters could be impeller configuration, vessel size, vessel type, number of baffles, etc. One core issue for this type of optimization problem is that 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 very 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 fulfil profitability requirements, resulting in a significant competitive advantage while delivering a better quality product.

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

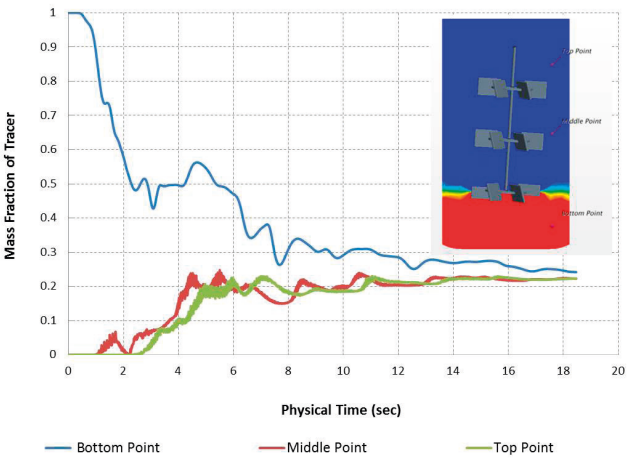

Figure 1A: Inert tracer method (resembling the widely used experimental technique) showing the quantitative change in local concentration as a function of time

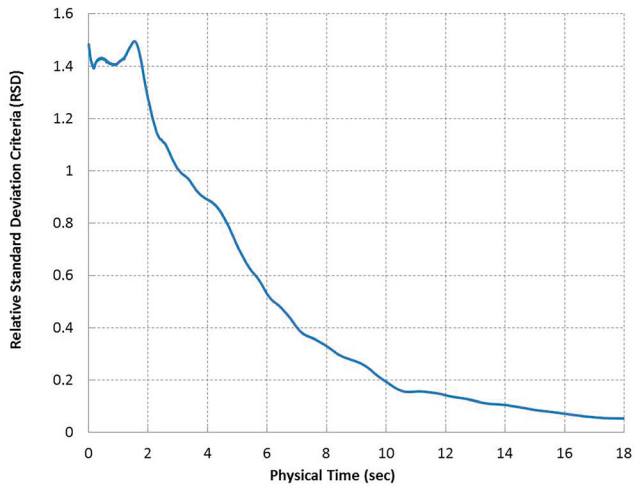

Figure 1B: Relative standard deviation method

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 non-dominated 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 non-dominated 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 vs. mixing time
2. Impeller moment vs. 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 which will be addressed in the following section.

Mixing criteria

The mixing time can be defined as the time it takes to achieve a pre-defined 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% homogeneity is the time needed for the fluctuations of the tracer concentration to be less than 10% of the concentration that 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, STAR-CCM+® has the capability of defining a variety of desired mathematical formulations for measuring the mixing quality through field functions. Also, STAR-CCM+ allows us to define a homogeneity threshold which permits 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:

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

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 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 STAR-CCM+ using the 3D-CAD modeler (Figure 2A). Mixed liquid was tracked as a passive scalar which is initially at rest at the bottom of the tank (Figure 2B).

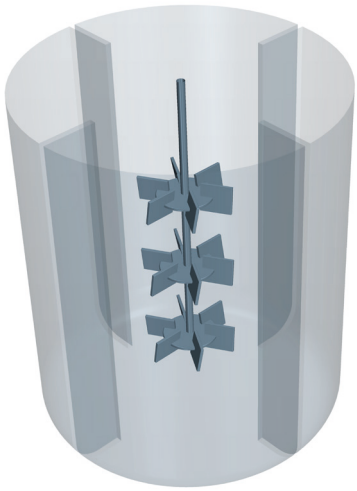

Figure 2A: Mixing tank geometry created in STAR-CCM+

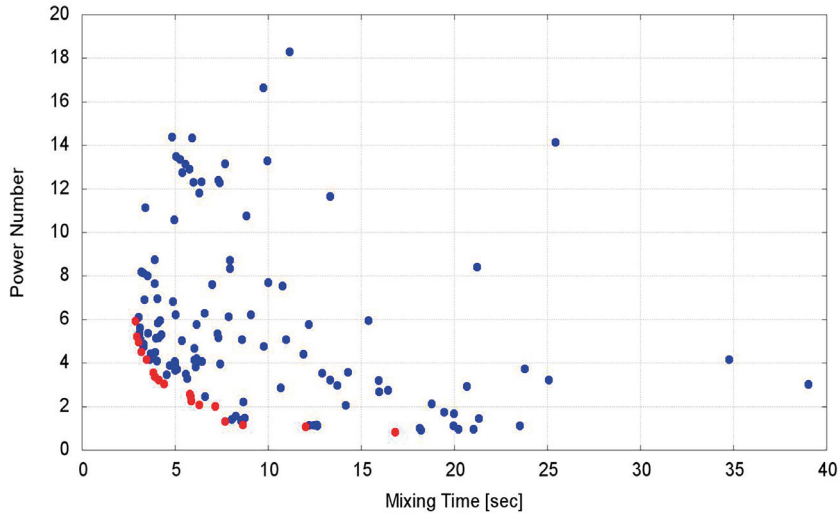

Figure 3: The results of Pareto front (red dots) show the designs forced by the optimizer to the optimal corner.

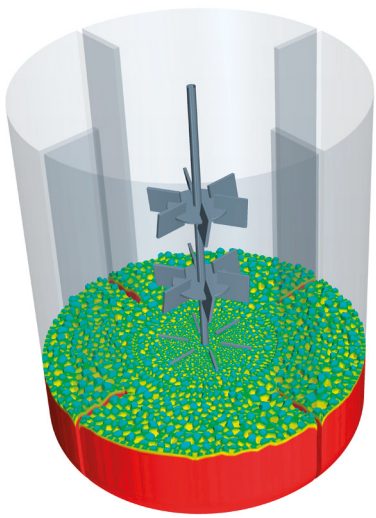

Figure 2B: The initial condition of tracers defined by Field Function

The Pareto front plot can provide the answer to the mixing industries 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?"

A transient simulation was performed using the Moving Reference Frame (MRF) approach. Here, the two competitive objectives being 1) power number vs. mixing time, and 2) impeller moment vs. mixing quality are discussed.

Competitive objectives 1: Power number vs. mixing time

Advanced CAD modeling capabilities in 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 division, Optimate has the choice for specifying the increment. For example, the increment for the number of impellers would be 1 (min=2, max=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

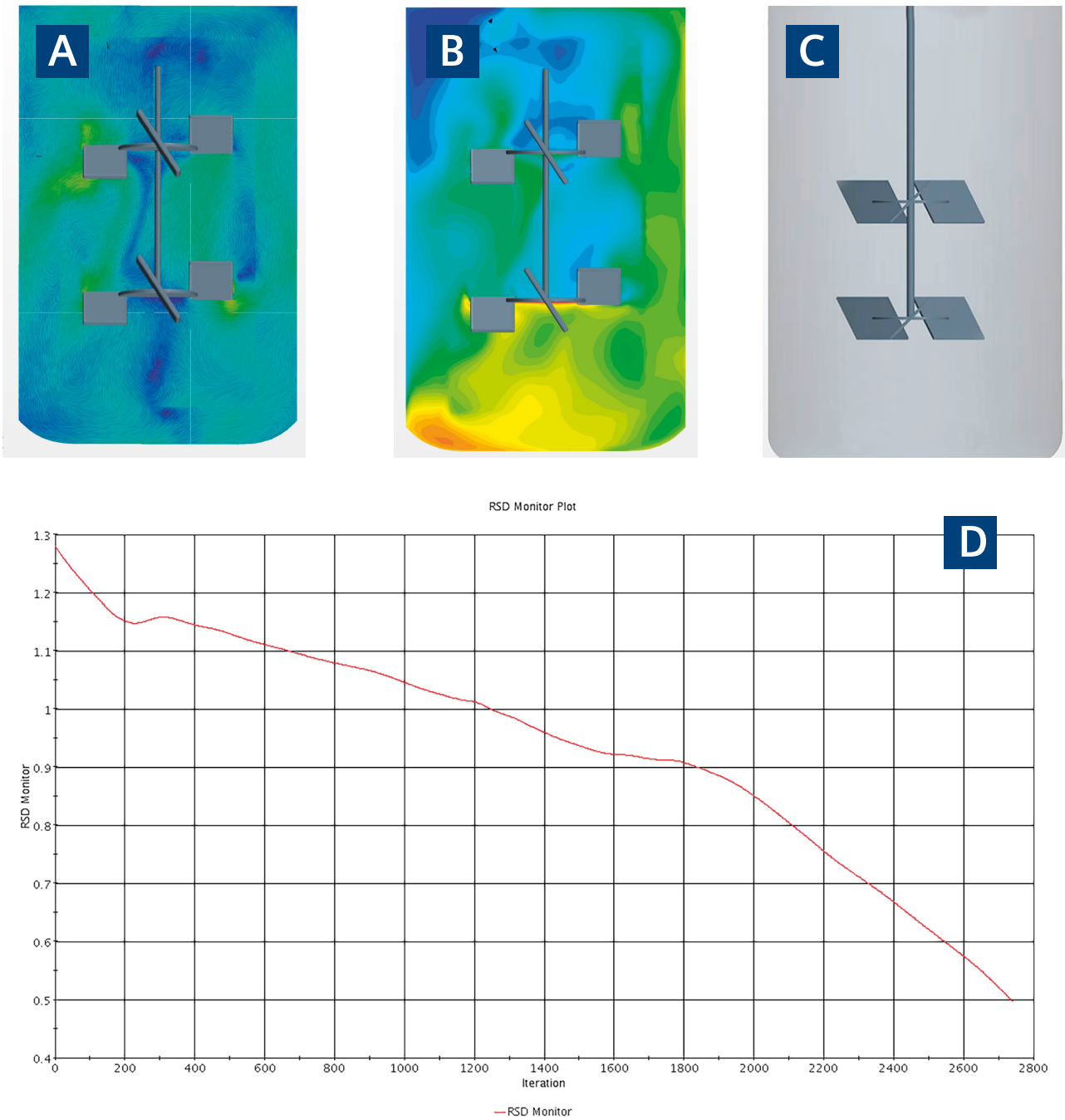

Figure 4: Velocity field (A), Tracer's mass fraction (B), CAD geometry (C), and RSD vs time (D) for one of the design points on the Pareto front

manually would be nearly impossible. Instead of running over eight 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 searching 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 100s 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

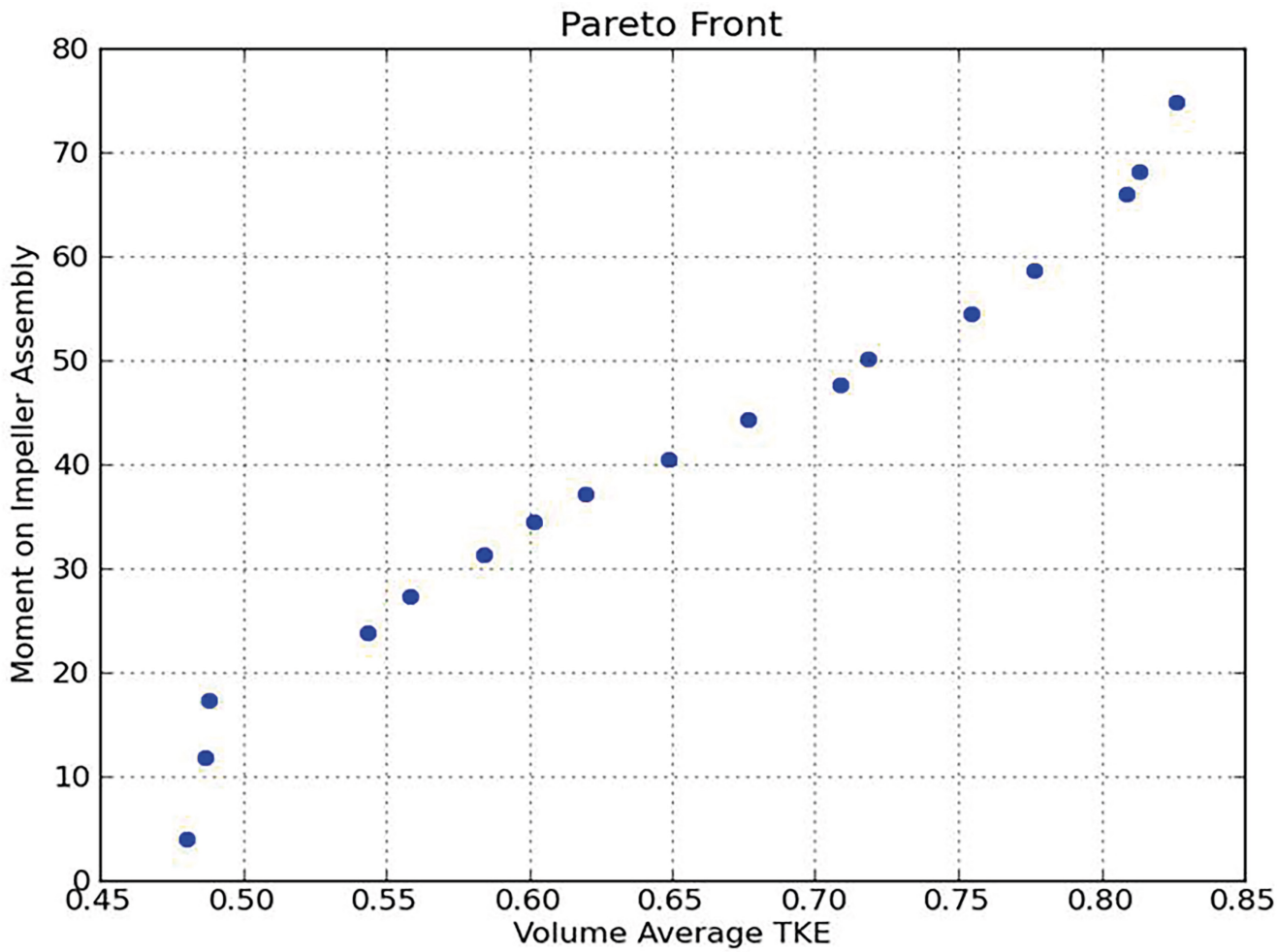

Figure 5: Pareto front for the moment on the impeller assembly vs. the volume-averaged TKE

Pareto front illustrates how the optimizer is forcing the designs towards the optimal corner which corresponds to lower values of mixing time and power number. 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 RSD-time plot as calculated by Optimate for one of the design points.

Competitive objectives 2: Impeller moment vs. 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 vs. power consumption, or moment on the impeller assembly vs. 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.

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 pre-defined set of operating conditions, ultimately resulting in savings worth millions of dollars.