Can Mixing Be Smart?

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Obtaining a pure product by mixing together raw materials, so as to carry out a chemical reaction at high selectivity, is a difficult part of manufacturing chemical products. How can we test reactors and mixers to ensure the efficient use of energy?

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In the chemical industry and related sectors, such as food, pharmaceuticals, cosmetics and plastics, the main goal is to convert raw materials into intermediate and final products with specific, precisely defined properties. The field of chemical engineering seeks to accurately interpret these processes. One interesting method involves the use of rotor-stator mixers to manufacture and formulate products. These types of mixers can generate high local values of mechanical stresses in selected regions of the device, while other regions can then be treated as passive with regards to stresses and mechanical energy consumption. This helps achieve high energy yield and efficiency of processes such as homogenization, dispersion, emulsification, grinding, chemical transformations, disintegration of microorganisms and coagulation. These processes are costly in terms of energy, thus the ability to predict its most efficient use is very valuable.

Providing a theoretical description of such a process, however, turns out not to be that simple. In

The Handbook of Industrial Mixing, Wiley, 2004, Atiemo-Obenga and Calabrese wrote: "the current understanding of rotor-stator devices has almost no fundamental basis." Many scientific articles have been published since 2004, including some written by the present author and Prof. Jerzy Bałdyga, which have described in detail how rotor-stator mixers work and the processes occurring within them.

Targeting the main product

Using a rotor-stator mixer to convert raw materials into a desired product is a complex, multi-stage process, which includes both mechanical and chemical aspects. The main problem with the chemical reactions is the possibility of creating by-products. In addition to the main product, unwanted products are created in quantities that depend on the conditions of the process. And yet the goal of the process is to, after all, create a pure product. One way to achieve this goal is to separate the main product from that mixture which also contains the by-products. This is, however, a very costly method in terms of energy. Another option is to conduct the process in a way that minimizes the production of by-products. When chemical reactions in homogeneous systems are concerned, the process of micro-mixing, or mixing on a molecular scale, plays a decisive role.

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On the other hand, if we are dealing with reactions taking place in two-phase liquid-liquid systems, the rate of mass transfer between the dispersed phase (drops) and the continuous phase can determine the selectivity of the process. Skillful control of methods applied to perform the processes and the rate of these processes, including mixing, mass transfer rates and the sequence of addition of reactants, can ensure that for any given reaction kinetics the process will lead to a clean product. Developing the respective methodology and implementation to enable mixing-controlled processes to be performed at high selectivity was one of the fundamental goals of the work done by our team.

Chemical reactions are classified as very slow, slow, fast or instantaneous, if their characteristic time constants are significantly higher, slightly higher, close to, or much lower than the mixing and mass transfer time constants, respectively. When a complex reaction system is involved, the main product is usually formed by a fast or very fast reaction, while the by-product results from a slow or very slow reaction. Thus, if the very fast or fast reactions are controlled by mixing, then it is the rate of mixing or mass transfer, not the chemical kinetics, that determines the rate at which the main product is created. The competition between the main reaction leading to the desired product and the side reactions comes down to the mixing versus the side-effects of chemical reactions. Very slow mixing will lead to side reactions, whereas quickly mixing the selected reagents together will lead to significant acceleration of fast reactions.

A mathematical modelling input

In industrial practice it has been observed that devices such as tank reactors with mechanical stirrers, or tubular reactors, do not provide sufficiently fast mixing. The alternative solutions that have been developed include micro-reactors and rotor-stator mixers. Due to their specific construction, these devices ensure fast mixing and mass exchange, and thus maximize the production of main products with controlled energy consumption. The energy efficiency and the cost of the process are closely related. Often, devices that allow fast mixing of reagents do not ensure efficient use of energy, which seriously increases the cost of the process. Experimental investigations have shown that both rotor-stator mixers and micro-reactors (although the latter to a much lesser extent) provide conditions allowing for the optimal use of energy. Favorable conditions for conducting complex chemical reactions in rotor-stator mixers and preferred mixer designs have been identified both during experimental studies and directly in industrial applications. The aim of our work, performed mostly in collaboration with Unilever and the University in Manchester, was to comprehensively study and describe the operation of rotor-stator mixers, by the use of scientific methods. This was to ensure the ability to predict the course of the process depending on the conditions used, and thus allowing the process and product to be controlled. Mathematical models were an essential research tool, with experiments serving to verify the modelling results.

Using advanced mathematical techniques, our models have succeeded in providing a systematic description of the mixing processes. These were mainly partial differential momentum balance equations (Navier-Stokes equations), species balance equations, and population balance equations. The latter made it possible to monitor the evolution of the distribution of the product particle sizes and its other properties. This is particularly important when a dispersed phase participates in the process, such as droplets, crystals or microorganisms. The balance equations mentioned above are the basis for modelling. However, they require the use of additional, specific models describing chemical kinetics, the rate of coalescence and drop breakage, as well as the rate of growth and aggregation of crystals, and many other rates of transformation of the dispersed phase. As mentioned earlier, the primary reason for conducting this research was to meet the needs of industry, especially in the context of producing pure products, but the results of our investigations ended up having enormous scientific value, mainly for understanding turbulent flows under high stresses, and determining the mixing and mass transfer mechanisms in such specific conditions. We also examined the influence of the flow, mixing, and mass transfer on complex chemical reactions.

Reducing energy waste

Chemical reactions are used primarily to produce valuable products in many industrial processes. However, some reactions, in particular complex reactions, are also used in scientific studies as indicators of specific mixing and mass transfer characteristics; we used them in this way in our work as well. As mentioned earlier, the final composition of output products depends to a large extent on the reagent mixing method used. Based on the composition of products, one can define mixing indices, and identify time constants of mixing and mass transfer processes. In connection with the above, we proposed a new, original method of using test reactions to identify the energy efficiency of a given process, offering a way to determine what part of the mechanical energy supplied to the system and dissipated in it is used directly to produce the product, and which is spent uselessly, and even to the detriment of the product. As a result, the method proposed by us makes it possible to compare, in terms of energy costs, the manufacture of products using such different devices as micro-reactors and rotor-stator mixers, and to compare such various processes as micro-mixing and dispersion of droplets in relation to mass transfer.

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Photography by **Jakub Ostałowski**

Further reading:

Bałdyga J., Kowalski A.,Cooke M., Jasińska M. (2007). Investigation of micromixing in a rotor-stator mixer. *Chemical and Process Engineering*, 28, 867–877.

Jasińska M., Bałdyga J., Cooke M., Kowalski A. (2013). Application of test reactions to study micromixing in the rotor-stator mixer (test reactions for rotor-stator mixer). *Applied Thermal Engineering*, 57 (1–2), 172–179.

Jasińska M., Bałdyga J. (2014). *Effects of Rotor-Stator Mixer Performance on Drop Dispersion, Micromixing, Mass Transfer and Chemical Reactions*. LAP Lamber Academic Publishing, Saarbrucken, Germany.