Mixing and Age Distribution in Chemical Reactors: 50 Years after Danckwerts and Zwietering

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Abstract

In his 1953 paper, Danckwerts formed foundation for residence time distribution. Today, RTD theory has been widely used in analyzing chemical reactor performances but several limitations restricted the theory for mixing quantification. In his 1958 paper, Danckwerts proposed the concept of degree of segregation. In 1959, Zwietering further discussed the concept and called it the degree of mixing. In the following fifty years, this concept has been widely accepted by mixing community and repeatedly mentioned in publications in chemical engineering journals but there has never been a method developed to calculate this measure for general chemical reactors.

In this talk, a new theory based on mean age and higher moments of age distributions will be discussed. This theory forms a new frame work for characterizing mixing processes in chemical reactors using CFD. Most of the limitations in the RTD theory are now eliminated by this theory. The degree of mixing can now readily be computed. The theory answers many other key questions that can not be answered with the currently available methods.

The mean age and higher moments of age are all governed by conservation equations in the same form as N-S equations and can all be treated as passive scalars. The current CFD solvers can then easily be used for solutions after velocity solutions are obtained. From numerical point of view, the solution process of these moments is extremely efficient compared to that for residence time distribution.

Mean age and the higher moments of age are closely related to the RTD. From the solution of mean age, inefficient design of a reactor, such as dead zones, short circuiting paths, etc., can easily be identified and characterized quantitatively. Such defects in reactor design can only be inferred or guessed using RTD theory.

With the solutions of mean age and the second moment of age, the degree of mixing can be computed for a steady continuous reactor. Three variances are defined. The relations of these variances explain why RTD theory can only show the closeness of a mixing process to an ideal mixer but not quantify the mixing status. These variances also reveal a new dimension in mixing analysis, mixing in time or age, in comparison with mixing in space. The state of this temporal mixing can be measured by one of the variances. This new measure is important for some bio reactors where cell age distribution is a key factor of the process. Applications of these variances to quantify mixing in continuous reactors will be discussed.

Mean age distribution also offers an extremely efficient method in calculating blend time in a stirred tank reactor. In the last two decades, there have been several occasions that CFD was attempted to compute blend time with RANS model but the reported results have been poor. More recently, LES has been used to compute the time dependent flow solution and tracer history. Good results in blend time predictions have been reported but the huge CPU time demanded by the computation is still an obstacle for the method to be used in industrial reactor design. Now with the mean age method, blend time can be computed in with a CPU time of orders of magnitude shorter than that of even the current RANS methods. The predicted blend times are in excellent agreement with correlations in literature. This method will enable CFD to become a reliable tool for industrial reactor design and scale-up.