

Introduction to Computational Fluid Dynamics for Multiphase Flows

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I. INTRODUCTION

In the process industries the conversion of raw materials to desired products via physical and/or chemical processes is of great significance and very often multiphase systems are involved. In the traditional chemical reaction engineering approach knowledge elements from physics (like fluid dynamics and transport theories), chemistry (kinetics, catalysis) and mathematics have been integrated to form powerful dedicated (empirical) tools which in combination with careful experimentation enable scientists and engineers to tackle extremely complicated problems that come up in studying and developing these processes. An emerging tool is a combination of fluid dynamics and numerical mathematics backed up by the immense growth of computer power: Computational Fluid Dynamics (CFD). It is expected that the traditional (empirical) approach will gradually be replaced by a CFD-based approach backed-up by (fewer) experimental studies. In the next section the traditional chemical reaction engineering approach will be discussed together with its relation to the CFD-based approach. Thereafter the CFD-based approach will be detailed followed by a discussion of computational examples for a number of important types of multiphase flows highlighting present capabilities and limitations.

II. TRADITIONAL APPROACHES

As mentioned earlier, in the past many powerful tools with a strong empirical base had been devised by chemical engineers to (approximately) solve extremely complicated problems encountered in chemical reaction engineering such as the design of process equipment (including chemical reactors) involving non-ideal flow (see Figure 1; Levenspiel, 1962). Very often the two idealized flow patterns, that is, plug flow and mixed flow, do not occur in reality but nevertheless these concepts have proven valuable when dealing with the design of chemical reactors because the conversion obtained in these two extreme cases provides the boundaries for the conversion in a chemical reactor in which non-ideal flow prevails. Levenspiel (1962) stated that “If we know precisely what is happening within the vessel, thus if we have a complete velocity distribution map for the fluid, then we are able to predict the behavior of a vessel as a reactor. Though fine in principle, the attendant complexities make it impractical to use this approach.” This situation has clearly changed because nowadays the “complete velocity distribution map” can in principle be obtained by computing the velocity distribution in the system of interest. A well-known traditional approach adopted in chemical engineering to circumvent the intrinsic difficulties in obtaining the “complete velocity distribution map” is the characterization of non-ideal flow patterns by means of residence time distribution (RTD) experiments where typically the response of a piece of process equipment is measured due to a disturbance of the inlet concentration of a tracer. From the measured response of the system (i.e., the concentration of the tracer measured in the outlet stream of the relevant piece of process equipment) the differential residence time distribution $E(t)$ can be obtained where $E(t)dt$ represents the fraction $dF(t)$ of the volume elements with a residence time between t and $t+dt$:

$$dF(t) = E(t)dt \quad (2.1)$$

The fraction of the fluid elements with a residence time of less than t is given by the cumulative residence time distribution function $F(t)$ given by:

$$F(t) = \int_0^t E(t) dt \quad (2.2)$$

For a continuous reactor with a non-ideal flow pattern, characterized by the differential residence time distribution $E(t)$, the following expression holds for the conversion $\xi_{\text{non-ideal}}$ (or any other relevant physical or chemical property) which is attained in case complete segregation of all fluid elements passing through the reactor can be assumed:

$$\xi_{\text{non-ideal}} = \int_{t_{\min}}^{t_{\max}} \xi_{\text{batch}} E(t) dt \quad (2.3)$$

where ξ_{batch} represents the conversion attained in a batch reactor with batch time t . Of course, in reality a certain degree of mixing between the fluid elements passing through the reactor occurs with simultaneous chemical transformation and therefore information on the macro-mixing patterns is generally not sufficient to enable accurate prediction of the extent of chemical conversion in a reactor possessing a non-ideal flow pattern. This mixing phenomenon necessitates the use of a micro-mixing model to account for the finite rate with which segregated fluid elements eventually achieve mixing at the molecular level (i.e., segregation decay) to permit the occurrence of a chemical transformation. Due to the advent of CFD the aforementioned approach can still be followed but now the $E(t)$ and $F(t)$ functions can in principle be obtained from the computed velocity distribution. Alternatively the species conservation equations can be solved simultaneously with the fluid flow equations and thereby the extent of chemical conversion can also be obtained directly without invoking the concept of residence time distribution.

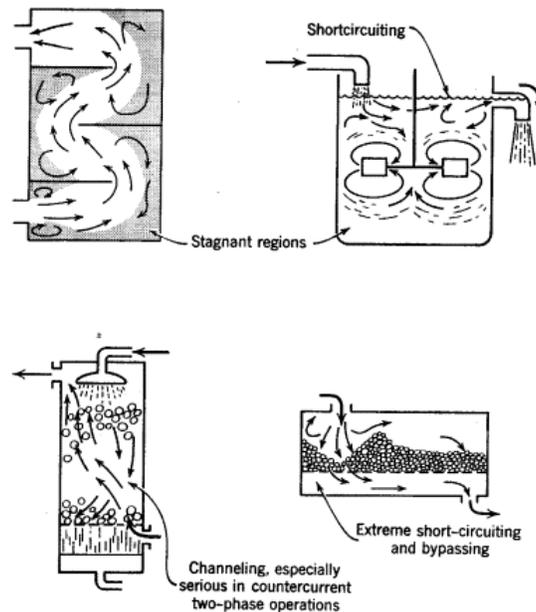


Figure 1: Some typical examples of non-ideal flow patterns that can occur in process equipment.