A First Course on Kinetics and Reaction Engineering
Unit 36. Segregated Flow Models

Overview

Segregated flow models, the focus of Unit 36, are an alternative to the ideal reactor models that can be used in situations where the flow assumptions of the ideal models are not met. Segregated flow models effectively represent the reactor as a distribution of smaller reactors. The distribution is chosen so that the residence times of the smaller reactors match the residence time distribution of the real reactor being modeled.

Learning Objectives

Upon completion of this unit, you should be able to define, in words, the following terms:
- micro-mixing
- macro-mixing

Upon completion of this unit, you should be able to write the defining equation for the following quantities:
- average value of a reactor variable that depends upon the residence time

Upon completion of this unit, you should be able to perform the following specific tasks and be able to recognize when they are needed and apply them correctly in the course of a more complex analysis:
- Describe the assumptions that are made in the segregated flow model.
- Discuss the difference between early mixing and late mixing segregated flow models.
- Perform reaction engineering tasks involving an isothermal reactor using a segregated flow model.

Information

Unit 11 described how the age function $F(\lambda)$ can be used to characterize the flow in a reactor. You may recall that $F(\lambda)$ is defined as the fraction of the fluid leaving a flow system at any instant that has been inside the system for a period of time less than λ. Unit 11 further showed how the age function could be measured experimentally by applying a tracer stimulus at the reactor inlet and then measuring the tracer response at the reactor outlet. It was noted in that unit that the age distribution function, $dF(\lambda)$, represents the fraction of the fluid leaving the reactor that has been inside the reactor for the differentially small interval of time, $d\lambda$, between λ and $\lambda + d\lambda$. The age function, $F(\lambda)$, and the age distribution function, $dF(\lambda)$, are related according to equation (36.1).

$$dF\left(\lambda\right) = \frac{dF}{d\lambda} d\lambda \qquad\qquad (36.1)$$

In cases where an *isothermal* reactor does not obey one of the ideal reactor models, it is possible to construct a model for the reactor that is based upon the measured age distribution function for that reactor. To do so, one assumes (or pretends) that as it enters the reactor, the fluid feed stream is divided up into very small, equally sized volumes of fluid called fluid elements. One further assumes that during

the entire time a fluid element is inside the reactor (a) it never mixes with any other fluid element and (b) there is perfect mixing within that fluid element. The perfect mixing *within* the fluid elements is sometimes referred to a micro-mixing, while mixing *between* fluid elements is referred to as macro-mixing. The segregated flow model is equivalent to assuming that the feed entering the reactor is split up (segregated) and placed into tiny little batch reactors where it remains until that batch reactor (fluid element) leaves the actual reactor. After leaving the actual reactor, the fluid elements macro-mix. Since the fluid elements do not macro-mix until after the fluid leaves the reactor, this model can be designated as a late-mixing segregated flow model.

The second assumption of segregated flow models is that each fluid element entering the reactor spends a unique amount of time inside the reactor before it leaves the reactor. Different fluid elements do not remain in the reactor for the same amount of time. Instead, it is assumed that the time spent in the reactor by the fluid elements is distributed among them according to the age distribution function. Thus, the fraction of the fluid elements that remain within the reactor for a period of time between λ and $\lambda + d\lambda$ is equal to $dF(\lambda)$.

The fluid within each fluid element begins to react as soon as that fluid element enters the reactor, and it stops reacting when the fluid element leaves the reactor. Because the fluid elements leaving the reactor have been inside for different amounts of time, the compositions of the fluid elements leaving the reactor are all different. However, because any one fluid element is perfectly mixed, the composition of that element can be calculated as long as one knows the feed fluid composition (the initial composition in the fluid element) and the amount of time that fluid element was inside the reactor. To do so, one simply solves the batch reactor design equations for that one fluid element. The exact size of a fluid element is not known, so it is necessary to assume a fluid element volume as a basis. The final composition of the fluid element then can be calculated using the feed composition, the batch reactor design equations and the residence time of that fluid element. Because an arbitrary basis is used when solving the design equations, the resulting final composition should be expressed as an intensive variable such as a concentration or in terms of an intensive reaction progress variable such as the fractional conversion.

To summarize up to this point, if the residence time of one particular fluid element is equal to t', the batch reactor design equations can be used to calculate the concentrations, $C_i(t')$ of the species, i, in that fluid element or the conversion, $f_i(t')$ of a reactant, i, in that fluid element at the time it leaves the reactor. Since it is assumed that the time spent inside the reactor by the fluid elements is distributed according to the residence time distribution, the fraction of the fluid leaving the reactor that came from fluid elements with a residence time of t' is equal to $dF(t')$. If the total volumetric flow rate of fluid at the outlet of the reactor is equal to $\dot{V}$, then $\dot{V}dF(t')$ is the outlet volumetric flow rate of fluid that had a residence time equal to t', and $\dot{V}C_i(t')dF(t')$ is the outlet molar flow rate of species i that had a residence time equal to t'. The total outlet molar flow rate of species i must then equal the sum of the outlet molar flow rates of species i with all possible residence times (that is, the sum from $F = 0$ to $F = 1$, or equivalently, the sum from $t' = 0$ to $t' = \infty$). Since the distribution of residence times is continuous, this sum takes the form of an integral as shown in equation (36.2), where the integration is over F, or equivalently in equation (36.3)

where the integration is over t'. The bar over the outlet molar flow rates in equations (36.2) and (36.3) indicates that they are averages over the distribution of fluid element residence times.

$$\bar{n}_i = \int_{F=0}^{F=1} \dot{V} C_i(t') dF(t') = \dot{V} \int_{F=0}^{F=1} C_i(t') dF(t') \tag{36.2}$$

$$\bar{n}_i = \dot{V} \int_{t'=0}^{t'=\infty} C_i(t') \frac{dF(\lambda)}{d\lambda}\bigg|_{\lambda=t'} dt' \tag{36.3}$$

The concentration of species i in the reactor outlet stream can be found by dividing equation (36.3) by the volumetric flow rate, equation (36.4). In fact, for any intensive property of the fluid that depends upon the fluid residence time, the average value can be found by integration over the residence time distribution. To do so, the property of interest, as a function of residence time, is multiplied by the residence time distribution and integrated over all possible residence times. For example, equation (36.5) can be used calculate the average residence time of all fluid leaving the reactor, and equation (36.6) can be used to calculate the outlet fractional conversion of species i according to the late-mixing segregated flow model.

$$\bar{C}_i = \frac{\bar{n}_i}{\dot{V}} = \int_{t'=0}^{t'=\infty} C_i(t') \frac{dF(\lambda)}{d\lambda}\bigg|_{\lambda=t'} dt' \tag{36.4}$$

$$\bar{t} = \int_{t'=0}^{t'=\infty} t' \frac{dF(\lambda)}{d\lambda}\bigg|_{\lambda=t'} dt' \tag{36.5}$$

$$\bar{f}_i = \int_{t'=0}^{t'=\infty} f_i(t') \frac{dF(\lambda)}{d\lambda}\bigg|_{\lambda=t'} dt' \tag{36.6}$$

It is important to note that equations (36.2) through (36.6) all assume that the age function has been properly normalized. The integration of a properly normalized age distribution function over all possible values of F, equation (36.7), or equivalently, over all possible values of t', equation (36.8), should equal 1.

$$\int_{F=0}^{F=1} dF(t') = 1 \tag{36.7}$$

$$\int_{t'=0}^{t'=\infty} \frac{dF(\lambda)}{d\lambda}\bigg|_{\lambda=t'} dt' = 1 \tag{36.8}$$

The late-mixing segregated flow model is equivalent to a PFR where small amounts of fluid are withdrawn all along its length. Recall that a PFR is perfectly mixed in the radial direction, and that fluid residence time proportional to the axial distance into the reactor (the distance a differentially thick fluid element has moved into the reactor divided by the velocity at which that element is moving equals the

residence time). Thus, fluid removed at any distance along the reactor has been perfectly mixed for the whole time it was in the reactor, just as in the segregated flow model. If a fraction of the total inlet fluid equal to $dF(t')$ is removed at the axial position corresponding to a residence time of t' for all possible residence times, and the removed fractions are then all recombined, the net effect is exactly the same as the segregated flow model. This is shown schematically in Figure 36.1.
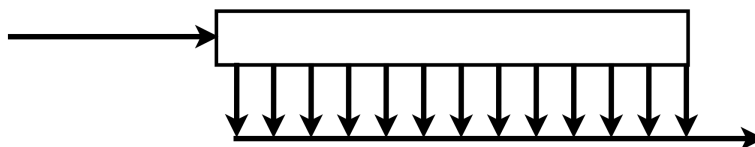

Figure 36.1. Schematic representation of the late-mixing segregated flow model in terms of a PFR. Fractions of the fluid flow are removed all along the length of the PFR in such a way that the residence times of the fractions removed matches the residence time distribution for the reactor being modeled.

It is possible to develop an early-mixing segregated flow model that retains the assumptions of segregation and perfect micro mixing, but where macro-mixing takes place as soon as possible. Consider the situation depicted in Figure 36.2. In that schematic the feed is admitted all along the length of a PFR, and again the fraction of the feed fluid admitted at any position, $dF(t')$, is chosen so that its residence time will equal t'. At each point where fluid enters, it is perfectly mixed with the fluid that is already in the reactor at that axial position. Like the late-mixing segregated flow model, this model assumes perfect micro-mixing, but unlike the late-mixing segregated flow model, macro-mixing occurs as soon as possible in this early-mixing segregated flow model.
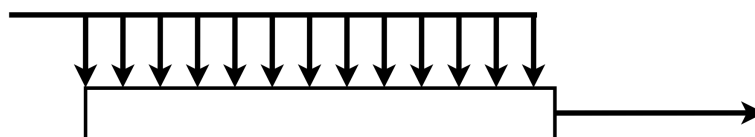

Figure 36.2. Schematic representation of an early-mixing segregated flow model that introduces macro-mixing as soon as possible.

Finally, it was mentioned near the start of this unit that segregated flow models could be formulated for _isothermal_ reactors that do not conform to the flow assumptions of ideal CSTRs or ideal PFRs. It would be much, much more complicated to extend the segregated flow models to a non-isothermal reactor. One would need to incorporate some way of deciding how much heat was transferred to each fluid element, whether heat was exchanged between fluid elements, if so, how much and at what rate, etc. etc. For these reasons, the segregated flow model is most useful for isothermal reactors, and non-isothermal reactors will not be considered in this unit.