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Nonideal Flow in Tubular Reactors

Stochastically Distributed Ideality

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Abstract

A compact and flexible method for modeling nonideal flow in tubular reactors is presented. The procedure involves dividing the reactor into discrete elements, each being an ideal reactor, but with characteristics of each assigned stochastically. Flow between cells is also shown as a stochastic behavior. The calculation steps are given in case of a fixed-bed reactor with unidirectional flow.

Index Entries: Nonideal flow, in tubular reactors; flow, nonideal, in tubular reactors; mass transport, in tubular reactors; tubular reactors, nonideal flow in; immobilized enzymes, in tubulor reactors; reactors, nonideal flow in tubular.

The aim of this presentation is to give a compact, yet flexible, method for describing nonideal flow in tubular reactors. Nonideal flow means flow deviating from plug flow. Only flow is considered, which means that the reaction itself is omitted from consideration—it may, however, be included easily. The tubular reactor is chosen since any reactor can be modeled as such using a nonideal flow pattern.

Two model types are currently available for describing nonideal flow (*1*):

1. Dispersion models.
2. Combined models.

In the first model type, a transport of mass against the flow direction (called dispersion) is included. When transients are considered, the general mathematical model becomes a number of partial differential equations that are not easily solved, and usually simplified cases are considered. In the second model type, combined

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models, a real reactor is modeled by establishing a network of elements, each being an ideal reactor, and combining these by appropriate flows (*1*, *2*). The method is somewhat lengthy in finding a well-fitting pattern of reactors, and the resulting model tends to be rather inflexible.

The model type to be described here is stochastic in nature, i.e., some features are described by probabilities, and basic parameters are not single numbers such as the dispersion coefficient in the dispersion model type, but instead probability functions.

To illustrate this mode of thinking, the modeling of a unidirectional flow in a fixed-bed reactor will be worked out. The model procedure consists of the following steps:

1. The reactor is divided into discrete "cells" of equal volume (see Fig. 1).
2. Void volume is distributed on individual cells according to a probability function being characteristic to the reactor given.
3. Flow changes between cell layers are formed by random recombination (to be explained in detail below).
4. The model is assembled.

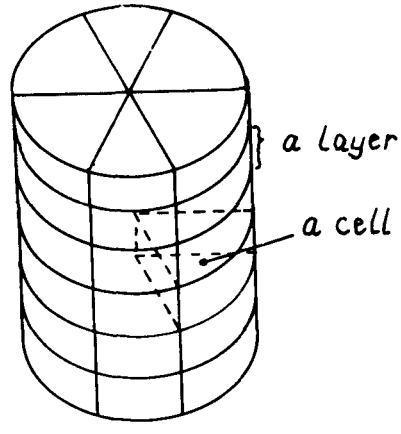

Fig. 1. The division of a tubular reactor into "cells" and "cell layers".

Step 1

Dividing the reactor into cells and unfolding it, the reactor will appear as shown in Fig. 2. The number of cells must be finite; usually 20–100 are used.

Step 2

Each cell is considered as an (ideal) plug-flow reactor with the void volume stochastically distributed according to a probability function that must be known in advance or found by fitting model output to pulse response curves. The probability function tells us that void volume is a given cell, ϵ_i, takes the value ϵ with a given probability p: $P(\epsilon_i = \epsilon) = p$. Using a Monto-Carlo procedure this probability function is used to assign a void volume to each cell.

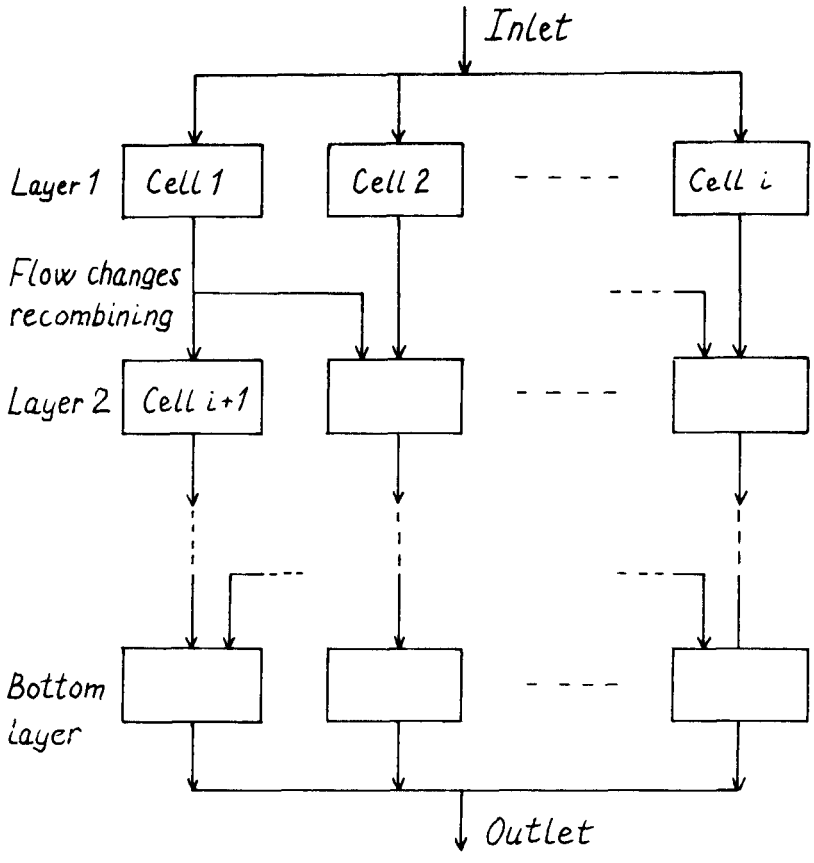

Fig. 2. Unfolding a reactor subdivided into cells.

Step 3

From isolated flow experiments, the flow dependence on void must be measured: $v = f(\epsilon)$. If the total inflow is called F, the flow in a given cell is then $v_i = (\alpha_i/\Sigma\alpha_i) \cdot F$ (the summing is across all cells in the layer to which cell i belongs). Since the outflow from one cell in general is different from the inflow to the cell after it, flows are split between layers (see Fig. 2). This recombination is done in a random fashion, although other ways of recombining may be applied if desired.

Step 4

Now the complete flow pattern in the column is known and response curves can be modeled by cell-to-cell calculations. At the outlet, the last layer outputs are pooled.

In the example given, unidirectional flow (not plug flow) in a tubular, fixed-bed reactor is described by combining plug-flow elements with voids assigned stochastically. The way of thinking presented may, however, include other flow directions or other ideal reactor types as elements. The basic characteristic is the

use of probability functions to distribute parameters on discrete subreactors (''cells'').

The features of the model type presented (tentatively called models with stochastically ideality) are:

1. Cracks, holes, plugging, channelling, air bubbles, etc., can be described.
2. Real tubular reactors may be described in terms of one measure: the probability function for the void distribution.
3. Complex reaction kinetics and flow resistance behavior can be incorporated in the cell-to-cell calculations employed.
4. Rather simple calculation is required.
5. The model is easily extendable to any reactor—not only the fixed-bed reactor—and to certain unit operations (extraction and filtration).

References

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