Optimize Reactor Networks using Gate and Highway Reactors and NEON

Novel methods for the systematic design of networks of conventional continuous flow reactors (Plug Flow Reactor: PFR and continuous Perfectly Mixed Reactor: PMR) for homogeneous constant density systems would be presented here.

It is found that the reactors are geometric objects in the Reaction Map. A Reaction Map is the space of concentration variables in which trajectories corresponding to the solutions of isothermal PFR equations have been plotted. A PFR corresponds to one such uni-dimensional curve. A PMR can be shown to be a tangent to some PFR trajectory. The PMR in an optimal network is shown to be an inflection tangent. The tangent point (Product) in the reaction map has been named as Gate and the starting point (Feed) is called Port. Such a PMR can be obtained from the equation:

$$\nabla\bar{r} \cdot \bar{r} = p\bar{r}$$

where $\bar{r}$ is the rate vector and p is an eigen-value of the matrix $\nabla\bar{r}$. Using this equation five problems involving single and multiple reactions have been solved.

Non-isothermal reactor network for van de Vusse reaction (A → B → C, 2A → D, Objective is to maximize the yield of B) has been obtained using the following observation:

$$B = \int \frac{dB}{dA} dA \le \int \left(\frac{dB}{dA}\right)^{*} dA$$

where $\left(\frac{dB}{dA}\right)^{*}$ corresponds to the extremum of $\left(\frac{dB}{dA}\right)$ which can be obtained by solving:

$$\frac{\partial}{\partial T}\left(\frac{dB}{dA}\right) = 0$$

The non-isothermal PFR corresponding to this equation has been called “Highway reactor”. To access the Highway reactor one needs an “Approach Road” reactor network and to reach the desired conversion an “Exit Road” reactor network. It can be shown that these accessory networks are well known optimal isothermal reactor networks operating at the constraints on temperature. The solutions of non-isothermal reactor networks for reported cases of rate constants have been solved to get same as or better than the known results.

Optimization of nonisothermal Plug Flow Reactor (PFR) usually gives a continuous temperature profile. Implementation of such a continuous profile would require infinitely many heat exchangers along the wall of the PFR, which is quite difficult. Here “NEar Optimal Networks” (NEON) are shown to logically evolve from Optimal Temperature Profile (OTP). Consecutive reactions have been taken as illustrative examples.

NEON-0 is Optimal Isothermal Reactor (OIR) that establishes the maximum incentive for the continuous temperature profile. For consecutive reactions this figure turns out to be 10% for (1, 1) reactions (the numbers 1 and 1 are the orders of the corresponding reactions) and 15% for (0.5, 3) reactions. NEON-I is Multi-stage Isothermal Reactor (MIR) with optimum stage lengths and temperatures. It is found that 3 stages are required to recover 80% of differential improvement by optimal reactor over OIR. NEON-II is Multi-stage Jacketed Reactor (MJR) with piecewise continuous linear temperature profile. NEON-II approaches real reactor having performance better by 1% than the corresponding MIR.

An approximate but fast method is proposed to calculate all the NEONs from OTP.