TECHNIQUE AND ALGORITHM FOR SELECTING A MIXING REACTOR FOR GAS–LIQUID REACTIONS

A. E. Kruglik

The principles of a technique and algorithm have been described [1] for choosing the type and optimizing the design of a bubble reactor for gas–liquid reactions which were used in developing hollow and sectioned column liquid-phase oxidizers for hydrocarbons. The technique and algorithm are based on a system analysis of the processes, in which the system is decomposed into hierarchical levels, the processes are formalized, mathematical models of the levels are synthesized, and the model is solved numerically using an efficiency function. At the microlevel the reactor type was chosen by minimizing the energy cost as a function of the chemisorption conditions. At the macrolevel the operational and design parameters were determined by maximizing the reactor efficiency. Here the principles of the technique and algorithm are used for the engineering selection and design of mixing-tank reactors for gas–liquid and gas–liquid–suspension systems when the reaction occurs in the liquid phase.

If a semicontinuous or batch gas–liquid tank reactor is intensively agitated mechanically, the technique and algorithm for selecting and designing the reactor can be simplified by reducing them to relatively simple engineering calculations without solving the complete mathematical model numerically. With some assumptions, an intensively agitated tank reactor can be reduced to a microlevel model, and the model calculations can be done using only maximum process rates (without knowing the detailed reaction kinetics).

The essence of the technique, on which the calculational algorithm is based, is as follows: by knowing the chemisorption conditions in a model (a laboratory or pilot-plant reactor), and by observing the conservation of the chemisorption conditions in the prototype (an industrial reactor), an industrial process can be realized, which has the same efficiency as the laboratory or pilot-plant reactor model.

In order to realize the technique and algorithm, it is necessary to obtain a universal mathematical microlevel model for a semicontinuous or batch gas–liquid tank reactor with intensive phase mixing.

In its general form, the mathematical description of the gas–liquid process in a semicontinuous reactor with ideal phase mixing has the following form.

Material balance:

- gas phase

\[ G_{\text{g0}} - G_{\text{gyr}} - \left[ k_\alpha/(1 - \varphi) \right] (c^*_y r - c_r) V_t = 0; \]

\[ G_{\text{gyg}} + \left[ k_\alpha/(1 - \varphi) \right] (c^*_y g - c_i) V_l = 0; \]

- solid suspension phase

\[ \pm k_{1-\varphi} S_\delta (c^*_j - c_{ji}) = dc_j/dr \]

- liquid phase

\[ [k_\alpha/(1 - \varphi)] (c^*_r r - c_r) - r_r = dc_r/dr; \]

\[ \pm [k_\alpha/(1 - \varphi)] (c^*_y g - c_i) \mp r_i = dc_i/dr; \]

\[ \pm r_k = dc_k/dr; \]
\[ \pm r_{l-\phi j}(c_j^* - c_{li}) = dc_j/dr. \]

Thermal balance

\[ (1 - \varphi)\Sigma \Delta H_{f,k,j} - k_c S_c(t - t_\phi) = (C_p/\rho)(dt_i/dr); \]
\[ -G_c C_p c(t_\phi - t) + k_c S_c(t - t_\phi) \pm Q_{loss} = C_p \rho_c V_c (dt_c/dr). \]

where \( G \) is the flow rate; \( y \) is the molar fraction of gas-phase components; \( k_l \) and \( k_{l-s} \) are the mass-transfer coefficients of the liquid phase and the liquid-solid system; \( a \) and \( S \) are the specific areas of the gas and solid contact surfaces; \( \varphi \) is the gas concentration; \( c^* \) is the solubility of the gas-phase components in the liquid phase; \( V_l \) is the volume of the liquid or the suspension; \( V_g \) is the volume of the [cooling] jacket; \( \tau \) is the reaction time; \( \Delta H \) is the heat of reaction; \( t \) is the temperature; \( \rho \) is the density; \( C_p \) is the heat capacity; \( Q_{loss} \) is the thermal losses; \( r \) is the chemical reaction rate; subscripts: \( r \) is for the gas reaction component; \( j \) and \( i \) are for the solid or liquid components; \( k \) is for the liquid-phase reaction product; \( c \) is for the coolant; 0 is at the inlet; "out" is at the outlet; and \( g \) is for the inert component of the gas.

The mathematical description of a batch reactor process is analogous to the above, but the right side of the material-balance equations for the gas phase has the form \( V_l (dY_r(g)/d\tau) \).

For the engineering technique for reactor selection, this system of equations can be simplified by using the following assumptions. The liquid-solid system is quasi-homogeneous, and the resistance at the liquid-solid boundary can be neglected, because the volumetric mass-transfer coefficient for the liquid-solid system is an order of magnitude or more larger than for the gas-liquid system for the overwhelming majority of gas-liquid processes with a solid suspension phase. Most batch chemical processes that include a gas phase occur at a constant pressure because the reaction gas is replenished; therefore the conservation equation for the gas phase is the same as for a semicontinuous process. As a rule, processes in a gas-liquid tank reactor are isothermal (at least for a selected portion of the reaction time).

Then the mathematical model is then simplified:

\[ G_{r0} - Gy_r - [k_r a((1 - \varphi))(c_j^* y_j - c_{rj})] V_l = 0; \]
\[ [k_r a((1 - \varphi))(c_j^* y_j - c_{rj}) - r_t = dc_t/dr; \]
\[ \pm [k_r a((1 - \varphi))(c_j^* y_g - c_i)] \mp r_i = dc_i/dr; \]
\[ \pm r_{j,k} = dc_{j,k}/d\tau; \]
\[ (1 - \varphi)\Sigma \Delta H_{f,k,j} - k_c S_c(t - t_\phi) = (C_p/\rho)(dt_i/dr) \rightarrow 0; \]
\[ -G_c C_p c(t_\phi - t) + k_c S_c(t - t_\phi) \pm Q_{loss} = C_p \rho_c V_c (dt_c/dr) \rightarrow 0, \]

The initial conditions at \( \tau = 0 \):

\[ y_r = 1, \ G_0 = G, \ G_g = 0, \ c_{i0} = 0; \]
\[ c_{i,j,k} = c_{0(j,k)}, \ t = t_0, \ t_{c,out} = t_{c0}; \]
\[ G_g i = \times r_i V_l, \ G = G_r + \Sigma G_g; \ y_r = G_r/[G_r + \Sigma G_r], \]

where \( x \) is the stoichiometric coefficient.

When the gas-liquid reaction occurs in a batch or semicontinuous reactor, the mass-transfer and reaction processes become quasistationary in time. Once the instantaneous process rate in the model (a laboratory or pilot-plant reactor) is known and the chemisorption conditions have been determined, the kinetic terms for mass transfer and the reaction can be corrected.