THE DYNAMICAL SYSTEM MODEL FOR REACTIVE DISTILLATION PROCESSES

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Introduction

1. Distillation (rectification) is one of the most common technological processes in the pharmaceutical industry. It is used for purification of chemical agents both after their synthesis and after solvent extraction.
2. The peculiar property of the pharmaceutical rectification is its subtlety related to the process temperature.
3. As a rule, drugs are sensitive to temperature: high temperature may result in drug destruction.
4. The differential dynamics model worked out here is applied for analysis of the processes in order to prevent destruction of the drug during its distillation but maintaining the high degree of purification.
5. The reactive distillation process is a distillation process complicated by spontaneous chemical reactions.

Coordinate System

Chemical engineering deals with n-component mixtures. We denote:
- $x_i$ - fraction of the $i$-th component in the liquid phase,
- $y_i$ - fraction of the $i$-th component in the vapor phase.

The homogeneous coordinate system is used, and the physical sense is realized only on ($n$-1)-dimensional simplex, $\Delta^{n-1}$.

Mathematical Model for the Reactive Distillation Process

The model for continuous reactive distillation is a nonlinear dynamical system:

$$\begin{align*}
\frac{dX}{dt} &= \beta(Y(X) - Y(X)) - \gamma Z(X) \\
\frac{dY}{dt} &= Y(X) - Y(X)
\end{align*}$$

where:
- $X$ is the vector of the liquid phase composition, $X = \{x_i\}_{i=1}^{n}$ ($1 \leq i \leq n-1$)
- $Y$ is the vector of the equilibrium vapor phase composition at its boiling temperature,
- $Z$ is the vector of the chemical reaction rate,
- $\beta, \gamma$ are constant scalar parameters of the system, $\beta > 0, \gamma > 0$.
- $\beta$ is the number of theoretical transfer units – the dynamical parameter, which is proportional to the height of the rectification column.

The mapping $Y = Y(X)$ is generally highly nonlinear. The thermodynamic restriction on the mapping can be formulated as the positive eigenvalues of its Jacobian matrix:

$$J(X) = \frac{dY}{dX}$$

Assumptions of the model:
1. The height of the theoretical transfer unit is the same for all components of the mixture and it is independent of the mixture composition.
2. Chemical reactions proceed only in the liquid phase.
3. Both the heat balance and the chemical reaction heat can be ignored.
4. The ratio between the molar flows of the liquid and gas phases in the column section remains constant.
5. The separation efficiencies of the cooler and the evaporator are equal to zero.

Obstacles for the Technological Processes

(i) The stationary points of the node-type of the dynamical system (1).
(ii) ($n$-1)-dimensional separating manifolds of the system.

This is why the emphasis is made on the problems of topological structure of the mathematical state space but not on the stability of the stationary states like in the traditional applications of dynamical systems.

Primary Objectives

1. Investigation the topological structure of the mathematical phase space (coupled concentration simplex) to the topologically connected domains.
2. Investigation of the variation of the topological structure due to varying the parameters.

Dynamical System in 2D Case

The most demonstrative case of the nonlinear reactive distillation model is the case of binary mixture. Then the model (1) is reduced to:

$$\begin{align*}
\dot{x} &= \beta(f(x) - y) - \gamma(z(x)) \\
\dot{y} &= f(x) - y
\end{align*}$$

where

$$f(x) > 0; \quad z(x) > 0; \quad 0 \leq x \leq 1; \quad 0 \leq y \leq 1$$

Here the highly nonlinear function $f(x)$ is the thermodynamical dependence of the molar fraction of the volatile component in the vapor equilibrium phase on its fraction in the liquid phase.

For the general type of binary chemical reaction:

$$A \rightarrow B$$

The reaction equation is:

$$z(x) = k_1 (1-x)^\beta - k_2 x^\gamma$$

Stationary (Equilibrium) Points

Equilibrium points are the roots of the system (2):

$$\begin{align*}
\beta(f(x) - y) - \gamma(z(x)) &= 0 \\
f(x) &= y = 0 \\
z &= 0
\end{align*}$$

The Jacoby matrix of the system (4) is:

$$J(x) = \begin{bmatrix}
\beta f'(x) - \gamma z'(x) & -\beta \\
f'(x) & 1
\end{bmatrix}$$

Its characteristic equation is:

$$\lambda^2 - \lambda (\beta f'(x) - \gamma z'(x) + 1) + \gamma z'(x) = 0$$

The stationary point has at least one saddle sector.

1. It is a saddle in the case of both zero- and first-order chemical reactions, and a saddle-node in the case of the second-order reaction.

Stationary Points of the Reactive Distillation Model in the 2D Case

<table>
<thead>
<tr>
<th>Chemical reaction</th>
<th>Chemical reaction order</th>
<th>Coordinates of the stationary point ($x_i$)</th>
<th>Multiplicity of the characteristic root</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A \rightarrow B$</td>
<td>Direct $n_1$</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$B \rightarrow A$</td>
<td>Reverse $n_2$</td>
<td>0,1</td>
<td>1</td>
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</tr>
</tbody>
</table>

Residue Curve Maps of the Reactive Distillation Process at the Neighborhood of the Stationary Point – Simple Root Case:

| a, b | azateotic and azeotropic mixtures with a reversible reaction; |
| c, d | azateotic mixtures with an irreversible reaction to the right and to the left, respectively. |

Conclusions

1. The differential dynamics model can be used for qualitative mathematical analysis of reactive distillation processes in pharmacology.
2. In contrast to the stability problems of differential dynamics, ($n$-1)-dimensional separating manifolds of this system and the stationary points of node-type are of the primary interest because they are obstacles for the technological process.
3. The demonstrative case of the 2D system is investigated, and we proved that the stationary point has at least one saddle sector.
4. The effect of structurally stable saddle-node was discovered in the case of irreversible reactions in binary mixtures.