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Short Communication

Limit cycles that do not comprise steady states of chemical reactors

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ABSTRACT

It is possible that self-induced oscillations appear in chemical reactors, and that their range does not reach the steady state, although such state exists. To prove this, a cascade of tank chemical reactors coupled with mass recycle loop was tested numerically. The above-mentioned phenomenon is characterized by the location of the steady point out of the limit cycle in the phase portrait. This incident may be beneficial to the process, as low steady state does not have to exclude an independent increase of the conversion degree, despite being the only state and not generating oscillations.

1. Introduction

The methods of graphic presentation of dynamic phenomena are time series and bifurcation diagrams. In the case of oscillations, the methods also include the so called limit cycles on the phase portrait.

According to available research results, nowadays there is a customary conviction that there should be a steady point inside a limit cycle. If both such solutions are stable, then, depending on the initial conditions, the apparatus can work under the steady state or under the oscillation state (for example: [1] and [2]).

However, this does not always have to be the case. It may happen that the steady point may be set outside the limit cycle. This phenomenon was originally described for a tubular reactor in [3] and [4]. Experimental results of the phenomenon were described by [5]. In this work it was presented in the example of cascade of Continuous Stirred Tank Reactors (cascade of CSTR) (see [6] and [7]) with mass recycle. A large number of tank reactors in the cascade can also be applied to approximate a dispersed flow (see [8]). Recycle systems are commonly used in chemical processes, as they enable an increase of the conversion degree and the utilization of the heat from the reaction.

The conducted numerical calculations discussed in the paper indicate that for the assumed model presented below, the setting of the steady point outside the limit cycle takes place already in the case of 15 reactors. For a smaller number of reactors, this phenomenon rapidly disappears, and then the steady point is surrounded by the limit cycle. The explanation is that the picture visible on the phase plane is only a projection from multi-dimensional space. In the case of a tubular reactor, the projection is from infinitely dimensional space. Thus, we are dealing with a spatial continuum model with infinite number of its own properties. For a cascade consisting of n tank reactors, each of which is described by two state variables (concentration and temperature), we are dealing with $2n$ dimensional space. It is worth noticing that the discussed phenomenon could also occur for a cascade consisting of two tank reactors.

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Nomenclature

c_p	heat capacity, kJ/(kg K)
C_A	concentration of component A, kmol/m^3
Da	Damköhler number $(=\frac{V_R(-r_F)}{\dot{F}C_{AF}})$
E	activation energy, kJ/kmol
f	recycle ratio, $(=\frac{\dot{m}_f}{\dot{m}})$
$\dot{F}$	volumetric flow rate, m^3/s
$(-\Delta H)$	heat of reaction, kJ/kmol
K	reaction rate constant, 1/s
Le	Lewis number, $(=1+\frac{m_w c_{pw}}{m_m c_{pm}})$
m	mass, kg
$\dot{m}$	mass flow rate, kg/s
$(-r)$	rate of reaction, $(=KC)$, kmol/(m^{3}s)
R	gas constant, kJ/(kmol K)
t	time, s
T	temperature, K
V	volume, m^3

Greek letters

α	degree of conversion $(=\frac{C_{AF}-C_A}{C_{AF}})$
β	dimensionless number related to adiabatic temperature increase $(=\frac{(-\Delta H)C_{AF}}{T_F\rho c_p})$
γ	dimensionless number related to activation energy $(=\frac{E}{RT_F})$
Θ	dimensionless temperature $(=\frac{T-T_F}{\beta T_F})$
ρ	density $(=\frac{kg}{m^3})$
τ	dimensionless time $(=\frac{\dot{F}}{V_R}t)$

Subscripts

1	refers to first CSTR
f	refers to recycle loop
F	refers to feed
i	refers to number of reactor
m	refers to medium
n	refers to last CTRS
w	refers to reactor wall

2. The model

It was assumed in this paper that there are n identical pseudo-homogeneous adiabatic tank reactors coupled with the recycle loop (Fig. 1). The mathematical model for a single reactor is the following:

$$\frac{d\alpha_i}{d\tau}+\alpha_i=\alpha_{i-1}+(1-f)Da(1-\alpha_i)\exp\left(\gamma\frac{\beta\Theta_i}{1+\beta\Theta_i}\right) \tag{1}$$

$$Le\frac{d\Theta_i}{d\tau}+\Theta_i=\Theta_{i-1}+(1-f)Da(1-\alpha_i)\exp\left(\gamma\frac{\beta\Theta_i}{1+\beta\Theta_i}\right) \tag{2}$$

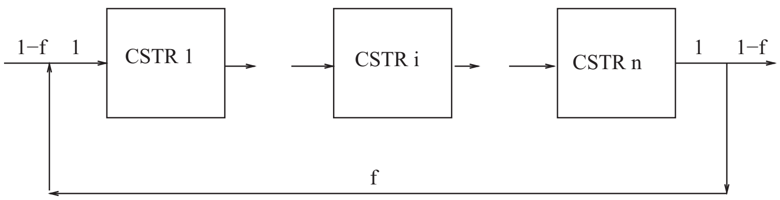

Fig. 1. Block diagram of the cascade of tank reactors.