

## Modeling and Simulation of the Industrial Processes Stability

Christo Boyadjiev

Institute of Chemical Engineering, Bulgarian Academy of Sciences, Bulgaria

### ABSTRACT

A theoretical analysis of the stability of the non-equilibrium industrial processes is presented. A unified approach is proposed for the creation of the mathematical models of the processes that allows the determination of the rates at which the processes move to their thermodynamic equilibriums and their use for mathematical analysis of processes velocities stability. For this purpose is used mathematical stability theory, evolution (autonomous) equations, bifurcation theory (stable focuses, stable cycles), parameter eigenvalues and eigenfunctions.

### \*Corresponding author

Christo Boyadjiev, Institute of Chemical Engineering, Bulgarian Academy of Sciences, Bulgaria. E-mail: chr.boyadjiev@gmail.com

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### Introduction

Non-equilibrium industrial systems are aggregations of physical, chemical and biological processes. They “move” to their thermodynamic equilibrium with a rate, that depends on the rates of the individual processes. Non-equilibrium industrial systems are stable when two conditions are met:

1. The rate of movement towards their thermodynamic equilibrium is a constant;
2. Capable of rapidly reaching their constant rate at deviations, as a result of smooth change of external conditions.

The theoretical analysis of the stability of the non-equilibrium industrial systems consists of 2 stages:

3. Creation a mathematical model of the system, allowing the determination of the rate at which the system moves to its thermodynamic equilibrium;
4. Mathematical analysis of system rate stability.

The first stage is different for individual systems, while the second stage is common to all industrial systems.

An unified approach will be proposed for the creation of a mathematical model of the system, which permits to be obtained the rate of the system movement to its thermodynamic equilibrium and mathematical analysis of the system stability.

### Chemical engineering processes kinetics

The kinetics of the chemical engineering processes depends on a set of variables. If the rate of these processes is denoted by the values of these variables, the equation of the kinetic model will have the form:

$$y = f(x_1, \dots, x_n). \quad (1)$$

This function is a mathematical structure that is retained when changed the measurement system of the variable, i.e. this mathematical structure is invariant with respect to similar transformations [1]:

$$\bar{x}_i = k_i x_i, \quad i = 1, \dots, n, \quad (2)$$

i.e.  $f$  is a homogeneous function:

$$ky = f(k_1 x_1, \dots, k_n x_n) = \phi(k_1, \dots, k_n) \cdot f(x_1, \dots, x_n), \quad (3)$$

$$k = \phi(k_1, \dots, k_n).$$

A short recording of (3) is:

$$f[\bar{x}_i] = \phi[k_i] f[x_i]. \quad (4)$$

The problem consists in finding a function  $f$  that satisfies equation (4). A differentiation of equation (4) concerning  $k_1$  leads to:

$$\frac{\partial f[\bar{x}_i]}{\partial k_1} = \frac{\partial \phi}{\partial k_1} f(x_i). \quad (5)$$

On the other hand

$$\frac{\partial f[\bar{x}_i]}{\partial k_1} = \frac{\partial f[\bar{x}_i]}{\partial \bar{x}_1} \frac{\partial \bar{x}_1}{\partial k_1} = \frac{\partial f[\bar{x}_i]}{\partial \bar{x}_1} x_1. \quad (6)$$

From (5, 6) follows

$$\frac{\partial f[\bar{x}_i]}{\partial \bar{x}_1} x_1 = \alpha_1 f[x_i], \quad (7)$$

where

$$\alpha_1 = \left( \frac{\partial \phi}{\partial k_1} \right)_{k_i=1}. \quad (8)$$

The equation (7) is valid for different values of  $k_i$  including  $k_i = 1$  ( $i = 1, \dots, n$ ). As a result  $\bar{x}_i = x_i, i = 1, \dots, n$  and from (7) follows

$$\frac{1}{f} \frac{\partial f}{\partial x_1} = \frac{\alpha_1}{x_1}, \quad (9)$$

i.e.

$$f = c_1 x_1^{\alpha_1}. \quad (10)$$

When the above operations are repeated for  $x_2, \dots, x_n$ , the homogenous function  $f$  assumes the form:

$$f = k x_1^{\alpha_1}, \dots, x_n^{\alpha_n}, \quad (11)$$

i.e., the function  $f$  is homogenous if it represents a power functions complex and as a result is invariant with respect to similarity (metric) transformations.

The parameters  $k, \alpha_1, \dots, \alpha_n$  are determined by experimental data of the industrial process rate. This allows to consider the rate of the industrial process  $y$  (phase rate) as a point in a  $n$ -dimension space, with coordinates  $x_1, \dots, x_n$  (phase space). Velocity projections

on coordinate axes  $x_1, \dots, x_n$  are  $\frac{dx_i}{dt}$  ( $i = 1, \dots, n$ )

and satisfy the “evolution” law of the industrial process:

$$\frac{dx_i}{dt} = a_i y = a_i k x_1^{\alpha_1} \dots x_n^{\alpha_n}; \quad t = 0, \quad x_i = x_{i0}; \quad i = 1, \dots, n, \quad (12)$$

where  $a_1, \dots, a_n$  represent the ratios of variable  $x_1, \dots, x_n$  velocities and the industrial process rate  $y$ .

The components of the phase rate  $\frac{dx_i}{dt}$  ( $i = 1, \dots, n$ ) are the coordinates

of the vector field at the same phase rate and determine the rate of motion of the industrial process in the phase space. The points  $x_i(t)$  ( $i = 1, \dots, n$ ) represent a curve (phase trajectory) in the scalar phase space.

If we use the rule to differentiate an exponent function, the derivative of the rate of the industrial process (4) over the time has the form:

$$\frac{dy}{dt} = k \prod_{i=1}^n [x_i(t)]^{\alpha_i} \sum_{i=1}^n \left[ \frac{dx_i}{dt} \frac{\alpha_i}{x_i(t)} \right]. \quad (13)$$

From this equation is possible to be obtained stability condition

$\frac{dy}{dt} = 0$  of the industrial process:

$$k \prod_{i=1}^n [x_i(t)]^{\alpha_i} \sum_{i=1}^n \left[ \frac{dx_i}{dt} \frac{\alpha_i}{x_i(t)} \right] = 0, \quad x_i(0) = x_{i0}, \quad i = 1, \dots, n. \quad (14)$$

The solution of this set of equations allows the determination of the conditions for the stability of the industrial processes.

### Mathematical Stability Theory

The rate of the non-equilibrium industrial processes with which they “move” to their thermodynamic equilibrium is determined by the theory of the evolution equations. Their capable of rapidly reaching their constant rate at deviations, as a result of smooth change of external conditions, is determined by the theory of bifurcations [2-5].

### Evolution Equations

Let consider the industrial process rate, which may be determined by the variables  $x_i$  ( $i = 1, \dots, n$ ). This permits to consider the state of the process as a point in  $n$ -dimensional space with co-ordinates  $x_i$  ( $i = 1, \dots, n$ ) (a phase space).

The changing of the process rate over the time is a vector in the  $n$ -dimensional space. Its projections on coordinate axes

$\frac{dx_i}{dt}$  ( $i = 1, \dots, n$ ) satisfy the “evolution” law of the process:

$$\frac{dx_i}{dt} = X_i(x_1, \dots, x_n, t), \quad x_i(0) = x_{i0}, \quad i = 1, \dots, n. \quad (15)$$

The evolution equations (15), for processes with laws independent of the time, are termed autonomous equations:

$$\frac{dx_i}{dt} = X_i(x_1, \dots, x_n), \quad x_i(0) = x_{i0}, \quad i = 1, \dots, n. \quad (16)$$

The components of the phase rate  $X_i$  ( $i = 1, \dots, n$ ) are the co-ordinates of the vector field of the same phase rate and determine the rate of the process in the phase space. The points  $X_i(t)$  ( $i = 1, \dots, n$ ) represent a curve (a phase trajectory) in the scalar phase space (field).

For simplicity of explanation consider the autonomous equation

$$\frac{dx}{dt} = X(x), \quad x(0) = x_0. \quad (17)$$

The process is stable when the system rate does not change over the time:

$$X(x) = 0, \quad (18)$$

i.e.

$$X(a) = 0. \quad (19)$$

It follows from (19) that the point  $x = a$  may be considered as a stationary point (the process rate is constant over time). If  $a = x_0$  it clear that

$$x(t) \equiv a \quad (20)$$

is a solution of (17), where  $a$  is a singular point.

For simplicity will be considered the linear version of the equation (17) and its solution:

$$\frac{dx}{dt} = \lambda x, \quad x(0) = x_0, \quad x = x_0 \exp(\lambda t). \quad (21)$$

It follows from (21) that  $x = 0$  is a singular point, i.e.  $x_0 = 0$  and the solution of (21) has the following features (see Figure 1):

$$\lambda < 0, \quad \lim_{t \rightarrow \infty} x(t) = 0, \quad \forall x_0; \quad (22)$$

$$\lambda = 0, \quad x = x_0, \quad \forall x_0; \quad (23)$$

$$\begin{aligned} \lambda > 0, \quad x = x_0, \quad \text{at } t = 0; \\ \lambda > 0, \quad \lim_{t \rightarrow \infty} x(t) \rightarrow \infty, \quad \forall x_0 > 0; \\ \lambda > 0, \quad \lim_{t \rightarrow \infty} x(t) \rightarrow -\infty, \quad \forall x_0 < 0. \end{aligned} \quad (24)$$

The multiformity of the solution at  $\lambda > 0$  is not a result of its non-uniqueness, but this due to the solution instability with respect of the small perturbation of the initial condition ( $x_0$ ).

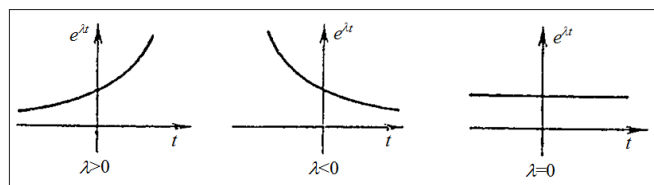


Figure 1: Solution of the equation (14)

The solution of the equation (14) leads to the following conclusions:

1. The solution (the process) is unstable at  $\lambda > 0$  and the small deviations of the initial state  $x_0 \neq 0$  lead to deviations of the solution  $x = 0$ .
2. At  $\lambda > 0$  the solution is unstable for each  $x_0$ .
3. At  $\lambda > 0$  the solution is approaching to the singular point  $x = 0$ , i.e. the stationary point become a focus of attraction of the solution (an attractor).

The linear equation (14), together with the conditions for the solution stability, are attractive because they give the basis of the kinetics models of many important processes (evolution of the organisms, nuclear processes, chemical reactions etc.) These features in the area of the real number ( $R$ ) become more interesting in the complex area ( $C$ ), where the equation (14) has the form:

$$\frac{dz}{dt} = \lambda z, \quad z \in C, \quad \lambda \in C, \quad t \in R, \quad z(0) = z_0, \quad z(t) = z_0 \exp(\lambda t). \quad (25)$$

### Bifurcation Theory

The bifurcation theory is wide applied for investigations of jump reactions of processes as responses of smooth changes of the external conditions. For the real processes it has been developed recently as a theory of the catastrophes. Here, the bifurcation theory will be considered in two-dimensional phase space only [5].

For clarity of explanation, consider that a real evolutionary process occurring in the phase plane ( $x, y$ ) and the corresponding model is:

$$\frac{dx}{dt} = X(x, y, \mu), \quad \frac{dy}{dt} = Y(x, y, \mu), \quad x(0) = x_0, \quad y(0) = y_0. \quad (26)$$

The process evolution in time is represented by the phase trajectory (the trajectory of the phase point) of the process

$$F(x, y, \mu) = 0, \quad (27)$$

where  $x(t)$  and  $y(t)$  in (27) are determined from the solution of (26). Depending on the form of the relationships for  $X$  and  $Y$  in (26), the parameter  $\mu$  and the initial conditions  $x_0$  and  $y_0$  various phase trajectories are possible.

The variations of the parameter  $\mu$  lead to several interesting cases of the solution of (26) shown in Figure 2. The case shown in Figure

2a corresponds to a periodic process that is attenuating with the time and approaching to a focus (a stationary state point). If other value of  $\mu$  is chosen the process might be unstable and periodic (Figure 2b). The stable periodic processes (limit cycles) have closed trajectories in the phase space (Figure 2c). The change of the initial state ( $y_0$ ) of the stable processes leads to attenuating processes approaching a stable periodic state. (Figure 2d).

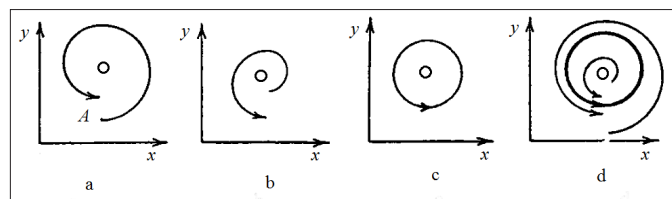


Figure 2: Phase trajectories

Figure 2 may be developed for more complicated cases (see Figure 3). It is possible the existence of two limit cycles (periodic processes and solutions), where one of them (the internal) is stable if the initial conditions are in the entire internal area of the large cycle. The internal cycle attracts all the solutions, while the external cycle is unstable (Figure 3a). The variations of the parameter  $\mu$  may lead to a junction of both cycles (Figure 3b). The junction of an unstable and a stable cycle (as these in Figure 3a) may lead to an abnormal limit cycle (Figure 3b). In this case the solutions go from the initial conditions in internal area, approach the cycle and then due to small perturbations may go out of the cycle, so the process becomes unstable. The further changes of  $\mu$  may lead to a situation when the limit cycle disappear and the process becomes unstable (Figure 3c).

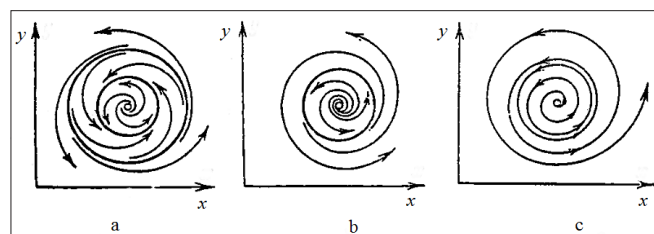


Figure 3: Limit cycles

The resulted obtained here show that the bifurcation theory considers qualitatively the changes of the movement of phase point as a result of a continuous variation of the model parameters. Parallel to the existence of stable points (focuses) there are stable cycles. They describe stationary periodic oscillations of the systems (self-oscillations). They differ from the free oscillations (of a pendulum for example) where the system does not interact with the environment as well as from the forced oscillations provoked by external periodic impacts.

The focuses and the limit cycles attracting the solution (the phase point) are termed *attractors*.

Figure 4 shows bifurcations of cycle transitions from focuses. The case (a) corresponds to a supercritical bifurcation (stable closed trajectories), while the case (b) presents a subcritical bifurcation (unstable and closed trajectories).

Further, Figure 4a shows the mechanism of a transition from a stable point (focus) toward a stable orbit (cycle). This type of bifurcation is shown in Figure 5. The stages of that transition are: 1) a stable point; 2) the occurrence of a closed trajectory; 3) an increase of the closed trajectory amplitude. This order leads to the existence of stable three-dimensional torus.

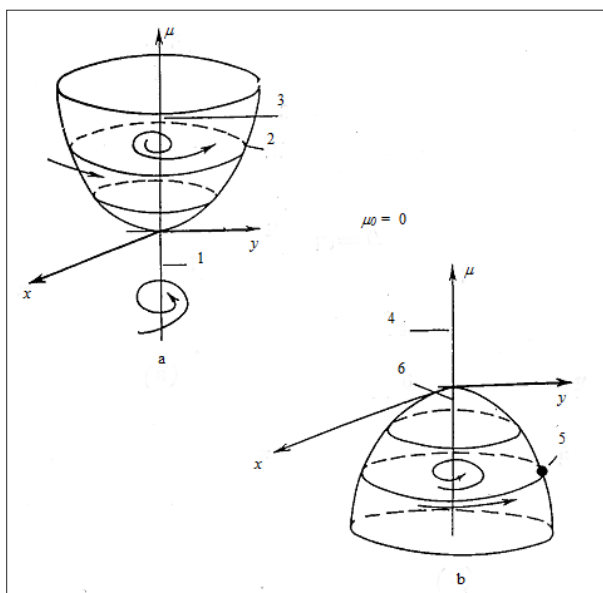


Figure 4: Bifurcation of cycle transitions from focuses

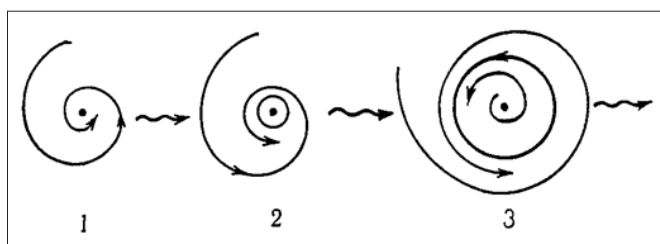


Figure 5: Mechanism of a transition from a focus toward a cycle

### Eigenvalue Problems

The presented analysis of the processes and the systems concerns its stabilities as functions of the model parameters. This requires a solution of differential equations with parameters. It is possible that the solution of the differential equation to exist at a given point (e.g. focus), only for a specific value of the parameter - "eigenvalue". For example, the second-order ordinary differential equation, when the boundary conditions are presented at two different points, can have solution for a specific value of the parameter only, i.e. this leads to eigenvalue problems. The solution to this problem will be demonstrated in a first order linear ordinary homogeneous differential equation:

$$y' + [f(x) + \lambda g(x)]y = 0, \quad (28)$$

where  $\lambda$  is a parameter and the solution must to satisfy the condition:

$$y(b) = \alpha y(a), \quad \alpha \neq 0. \quad (29)$$

The solution of (28) is well known

$$y = C \exp \left[ - \int_a^x (f + \lambda g) dx \right]. \quad (30)$$

The substitution of (30) in (29) shows that the condition (29) is satisfied, when  $\lambda = \lambda_0$ , only:

$$\lambda_0 = - \frac{\ln \alpha + \int_a^b f dx}{\int_a^b g dx}, \quad (31)$$

well known as an eigenvalue. The substitution of (31) in (30) leads to an eigenfunction. Thus, for example at  $f \equiv$  and  $g \equiv 1$  it follows directly:

$$\lambda_0 = \frac{\ln \alpha}{a-b}, \quad y = C \exp \left[ - \frac{\ln \alpha (x-a)}{a-b} \right]. \quad (32)$$

It is well demonstrated in the differential equation theory that if  $\int_a^b g dx \neq 0$  there is an infinite set of eigenvalues [6]:

$$\lambda_k = \lambda_0 + \frac{2k\pi i}{b-a}, \quad k = 0, \pm 1, \pm 2, \dots \quad (33)$$

The results obtained are used for the theoretical analysis of the hydrodynamics stability in systems with non-linear mass transfer [7].

### Conclusions

The presented theoretical analysis shows, that the stability of the non-equilibrium industrial processes (physical, chemical, biological and economic processes) is possible to be analyzed by the creation a mathematical model of the process, the determination of the rate at which the process moves to its thermodynamic equilibrium and mathematical analysis of process velocity stability.

A unified approach is proposed for the creation of the mathematical models of the processes that allows the determination of the rates at which the processes move to their thermodynamic equilibriums and their use for mathematical analysis of processes rates stability. For this purpose is used mathematical stability theory, evolution (autonomous) equations, bifurcation theory (stable focuses, stable cycles), parameter eigenvalues and eigenfunctions.

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