Methodology and Results of Mathematical Modelling of Complex Technological Processes

Nataliya V. Mokrova

1Moscow State University of Civil Engineering, Russia, Moscow, 129337, 26, Yaroslavskoye Shosse

Abstract. The methodology of system analysis allows us to draw a mathematical model of the complex technological process. The mathematical description of the plasma-chemical process was proposed. The importance the quenching rate and initial temperature decrease time was confirmed for producing the maximum amount of the target product. The results of numerical integration of the system of differential equations can be used to describe reagent concentrations, plasma jet rate and temperature in order to achieve optimal mode of hardening. Such models are applicable both for solving control problems and predicting future states of sophisticated technological systems.

1. Introduction

Today, any production process in any sector, be it engineering or construction or economic or social, could be considered as a complex process packed full of variables and connections. A scientific approach involves studying a wide class of related interconnected phenomena that obey certain laws, rather than a particular elementary process. By modelling, we mean a scientific cognition method aiming to analyze an object or a system of objects by building models and studying their essential properties identified in the mathematical description modelling process [1]. The modelling process, much less the practical application of mathematical and simulation models of complex systems, must be iterated numerous times, and at each stage its attributes are refined, modelling priorities are set and the ways to build newly built objects are rationalized. The mathematical description scheme obtained in the course of modelling together with the parameters identified as a result of interpolation, reflect the most essential features of the object or process and allow us to understand the mechanism of the phenomenon and make it possible to forecast changes in the phenomenon and its development trend. Different models, connections and relationships between individual components or subsystems, which are considered most relevant for this research, can correspond to the same process. They are written down using mathematical relations, which are checked for adequacy at the final stage of modelling, and, finally, the developed mathematical model is validated for accuracy and usability.

2. Methodology of complex technological processes modelling

Production processes in various industries have a number of features: they are mostly continuous and stochastic; chemical transformations and heat and mass transfer in technological processes depend both on the internal state of an object and external environment. The interaction of the object of research with the external environment is characterized by the loss of mass and energy and, therefore, by the process quality. To increase the efficiency of production, it is necessary to ensure optimal modes for individual processes and stability of external conditions.
Owing to the complexity of a specific technological process, for which a mathematical description is developed; the need for complex processing of raw materials; the need for rational use of energy and materials and recovery of side-line material and energy flows a systematic consideration of complex multi-stage processes characterized by homogeneous and heterogeneous stages in the chemical and related hi-tech industries will be necessary.

The system analysis is based on decomposition of a complex system into subsystems and establishment of quantitative relationships between such subsystems [2]. Subsystems (levels) are allocated not only depending on the complexity of the object under consideration, but also on the information about the object, previous study of process physical and chemical regularities, availability or possibility of obtaining a mathematical description of each stage [3]. If a subsystem with its I/O flows is considered independently, it is possible to estimate the potential of flows and subsystems and identify loss sources and ways to minimize such losses, and determine the reserve for increasing the efficiency of individual devices and the entire system.

The system analysis methodology applied in the development of a mathematical model of the generalized technological process is shown in Figure 1. The research proposes a mathematical description of the plasma-chemical process and fine purification of cobalt solutions from iron and copper.

The use of low temperature plasma in chemical engineering makes it possible to run processes at high temperatures and direct exposure to electric and magnetic fields and accomplish transformations that do not occur at all or are extremely time consuming (hundreds or thousands of times) under normal conditions [4-7].

### 3. Results of mathematical modelling of plasma-chemical processes

The analysis allows us to draw a conclusion about the prospects of complex processing of natural gas and other hydrocarbons in the plasma to produce coherent nitrogen, acetylene and hydrogen. The process is carried out at 2000°C and atmospheric pressure; methane pyrolysis is carried out in nitrogen plasma to produce simultaneously up to 10.5% of hydrogen cyanide and up to 13.5% of acetylene. It should be noted that methane pyrolysis carried out in a jet of hydrogen plasma at 4000°C can produce an acetylene concentration in the reaction products of up to 15.5% by volume, with a total degree of methane conversion reaching 85% and the ‘methane-to-acetylene’ conversion reaching 71.5% at a total energy consumption of 9.5-10 kWh per 1 m³ of acetylene.

A plasma-chemical plant is a sequence of a plasmatron, plasma-chemical reactor and a quenching device. A complete mathematical description of such plants is very sophisticated and requires knowledge of all the elementary processes occurring in the system at all levels. The plasmatron
mathematical model can be represented in the form of a system of partial differential equations comprising the following equations: material balance by components, mass continuity, pulse and quantity of motion conservation, plasmatron arc dynamics at minor arc deviations from its equilibrium state, and equation of state [8].

In practical modelling, a system of assumptions is applied, taking into account the most essential processes occurring in the system. The equations describing electromagnetic phenomena are not considered when describing the reaction node. Plasma-chemical process kinetics equations should be written down for all reacting components, and, at the same time, a simplified scheme of the mechanism of thermal decomposition of methane with the formation of acetylene at high temperatures should be developed and explained [8]. Write equations of reactions:

\[
\begin{align*}
2 \cdot CH_4 & \rightarrow C_2H_4 + 2 \cdot H_2 \\
C_2H_4 & \rightarrow C_2H_2 + H_2 \\
C_2H_2 & \rightarrow 2 \cdot C + H_2
\end{align*}
\]

(1)

Hydrodynamic phenomena play an important role in the description of acetylene formation processes, because the processes run in a flow reactor at high flow rate. It should be noted that the laws of an ideal gas are applicable to thermal plasma even at pressures on the order of 1000 atmospheres, because the density of plasma-forming particles is very small due to high temperatures.

The system of differential equations describing plasma-chemical processes is stiff. High temperatures, low reaction rates, exponential dependencies for the calculation of reaction rate constants (for example, the methane residence time in the reaction zone corresponding to the maximum yield of acetylene which equals to \(7.21 \times 10^{-4}\) seconds) complicate the search for a system solution by known numerical methods, and impose high standards on setting system parameters, refining ranges of coordinate variation; additionally, any additional experiment with the object of modelling is associated with certain technical and production difficulties.

It is important to note that the production of acetylene from hydrocarbons is a process where the final product is intermediate in the chain of reactions, therefore it is necessary to interrupt the reaction at the desired stage by quenching. It has been established experimentally that in order to produce the maximum amount of the target product we should focus on the quenching rate and initial temperature decrease time; it has been established that a \(2 \times 10^{-3}\)-sec quench delay leads to a 15.5 .. 10 % decrease in the acetylene concentration.

The importance of maintaining the optimum temperature profile throughout the entire technological process can be explained by the following: acetylene polymerizes vigorously at temperatures below 600°C to form solid and liquid substances; both decomposition and polymerization occur at 600-1000°C; a slow decrease in the gas mixture temperature leads to the decomposition of acetylene into hydrogen and soot, especially at 1200-1300°C. So, to quench plasma-chemical reaction products and shift the system to the temperature range on the order of 2000°C to make it stable for acetylene, a higher rate of mixture cooling will be necessary. The experimental studies and modelling results show that both intensive mixing of flows and dramatic uniform decrease in the temperature of reaction products can significantly increase the yield of the desired product.

The results of numerical integration of the system of differential equations obtained in the course of mathematical modelling of the plasma-chemical process can be used to describe what reagent concentrations, plasma jet rate and temperature should be opted for to achieve optimal quenching of reaction products. The analysis of changes in the concentration of reaction mixture components has revealed that the concentration of the initial substance - methane - decreases in time monotonously in accordance with the law of kinetics of simple reactions. Ethylene and acetylene concentration curves are described by an extremum dependence. The position of points of the maximum value of product concentration corresponds to the sequence of their formation. The temperature curve has an extremal form with a selected minimum point, which is reached in the interval of \(10^4-10^5\) seconds and almost coincides with the instant of formation of the maximum acetylene concentration; and reaching a minimum, the temperature begins to increase dramatically to make acetylene decompose at a growing rate. Forced quenching of the reaction mixture at the optimum time allows to prevent decomposition
of the target product and ensure a sufficiently high yield of acetylene. Modelling of plasma-chemical plants provides an opportunity for building systems that are able to help control the behavior of similar objects in an optimal way.

4. Mathematical modelling of purification processes

The system analysis methodology has allowed to solve the problem of modelling a multistage chemical and technological process of cobalt production [9, 10]. Cobalt solutions are purified in a cascade of 3 continuous reactors; primary products pass through the devices to react with caustic ash (main agent) with subsequent precipitation of iron and copper impurities and cobalt decline. The purification mathematical model is developed using the building-block concept.

The problem of optimal control over the purification process is formulated with a strict restriction with regard to the concentration of impurities. According the research chosen, methods for identifying a mathematical model of a cascade of reactors at the fine purification stage were proposed and a successive approximation method was adopted to identify the characteristics of the subsystems. When building a mathematical model of dynamics of the fine purification process, we used experimental data and coefficients obtained in the analysis of the process statics. The system of differential equations that characterize the dynamics of fine purification (decontamination) of cobalt solutions is described by the quartic Runge-Kutta method at a constant step. The analysis of dynamic processes in the cascade of reactors allows us to conclude that it is important to solve control tasks by means of the last reactor in the cascade as this helps control the set acidity value. Such models are applicable for solving control problems and predicting future states of systems.

5. Conclusion

Thus, in accordance with the system analysis methodology, the levels of the hierarchical structure of the system under consideration are distinguished for each of the technological processes considered in the research; we examined their interrelations, determined the aspects of their mutual influence, elucidated physical and chemical phenomena in each device and took into account characteristics of main state variables and controlling and disturbing influences. We put forward a mathematical description of the stages, which helped us find more rational ways of running the process and solve optimization problems. Such models are applicable both for solving control problems and predicting future states of sophisticated technological systems.

As already noted, the system analysis is based on decomposition of a complex system into subsystems and establishment of quantitative relationships between such subsystems. Subsystems (levels) are determined not only depending on the complexity of the object under consideration, but also on the information about the object, previous study of process physical and chemical regularities, availability or possibility of obtaining a mathematical description of each stage. If a subsystem with its I/O flows is considered independently, it is possible to estimate the potential of flows and subsystems and identify loss sources and ways to minimize such losses, and determine the potential for increasing the efficiency of individual devices and the entire system. A quantitative system analysis of complex chemical processes employing state-of-the-art computing facilities and mathematical modelling is necessary both for the development of new processes and intensification of existing ones.

References

[1] Lasdon L S 2011 Optimization Theory for Large Systems (New York: Dover Publications).

[2] Peregudov F I and Tarasenko F P 1989 Introduction to System Analysis (Moscow: High School).

[3] Mesarovic M D and Takahara Y 1975 General Systems Theory: Mathematical Foundations (Amsterdam: Elsevier Science).

[4] Polak L S 1975 Theoretical and Applied Plasma Chemistry (Moscow: Nauka).

[5] Polak L S and Lebedev Yu A 1991 Low-temperature plasma (Chemistry of Plasma vol 3) (Novosibirsk: Nauka).
[6] Polak L S and Lebedev Yu A 1998 *Plasma Chemistry* (London: Cambridge International Science Publishing).

[7] Hanz S N, Melnik A P and Parhomenko V D 1969 *Plasma in Chemical Technology* (Kiev: Tehnika).

[8] Artamonov A G, Volodin V M and Avdeev V G 1989 *Mathematical Modelling and Optimization of Plasma-chemical Processes* (Moscow: Himia).

[9] Mokrova N V and Volodin V M 2007 *Chem. Oil Gas Eng.* 2 17–9.

[10] Mokrova N V and Volodin V M 2006 *Bull. TSTU* 12 22–8.