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Mathematical principles of modeling processes of heat and mass exchange in multiphase media

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Mathematical principles of modeling processes of heat and mass exchange in multiphase media

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Abstract. The paper presents a method for studying the process of heat and mass transfer in multiphase media by the example of constructing mathematical models.

Modeling is a scientific method for studying complex technological processes or technical systems using models (physical or mathematical), which allows you to analyze the influence of structural and operational parameters of a process or system on their effectiveness.

The theory of modeling is developing in two directions:

1. Computational and theoretical research (usually using a computer) of mathematical models (mathematical description) of heat and mass transfer processes in multiphase mathematical modeling.
2. Experimental studies on material (physical) models - physical modeling [2].

In mathematical modeling, the object of study is an idealized mathematical model of the heat and mass transfer process in multiphase media, which is written as a system of differential equations with the corresponding initial and boundary conditions and establishes a relationship between the individual physical variables [2, 3].

Two approaches are used in mathematical modeling. One of them is the “black box” method (the Box method is one of the authors of the mathematical method of response surfaces). In this method, the object under study (for example, a chemical or energy reactor) is characterized only by external parameters - what enters into it and what exits from it. The mechanism of processes occurring inside the reactor is not deliberately considered. The optimal conditions for the process are determined by planning the experiment: varying the initial parameters, recording the “response” of the system, that is, changes in the resulting parameters, and, therefore, choosing the shortest path leading to the optimal mode.

However, the application of the Box method in its pure form to real objects is fraught with certain difficulties due to the variety of parameters that affect the processes of heat and mass transfer, and the complex nature of their influence. In addition, several different stationary modes can correspond to the same values of external parameters.

The second approach in mathematical modeling is based on a detailed analysis of the mechanisms of heat and mass transfer in multiphase media. When implementing this approach (let's call it deterministic), a system of differential equations is used that describes various "elementary" processes that make up the real work process of heat and mass transfer [5].

The most fruitful method of modeling heat and mass transfer is an integrated approach, including mathematical and physical modeling.

In mathematical modeling, the object of study is the equation - from the simplest algebraic to complex systems of nonlinear differential, integral or integro-differential equations. In the course of mathematical modeling, the physical model of the process is initially selected.

Then a system of equations is written, usually differential, with the corresponding boundary conditions describing the behavior of the model system (mathematical model), and a method for solving it, usually numerical, using computer technology is selected (in some cases, it is possible to obtain an analytical or asymptotic solution to the problem). Physical and mathematical models together constitute a physical and mathematical model of the studied process of heat and mass transfer.

The next stage of mathematical modeling is a series of calculations (mathematical experiment) for given ranges of changes in the determining parameters and analysis of the results [9].

The reliability of the developed physical and mathematical model is confirmed by conducting control experiments at several characteristic points in the region of the process under study.

The effectiveness of mathematical modeling can be estimated by analyzing the entire chain of heat and mass transfer processes. Let us consider the main elements of this chain (the choice of a physical and mathematical model and numerical algorithms) using the problems of continuum mechanics as an example. For these problems, in the most complete formulation, physical and mathematical models can be described by integral conservation laws expressing the relationship between the time variation in a closed volume V_0 of some quantities (flows) W_0, W and their change when crossing the border, as well as the interaction of flows with external sources or threads F:

$$\frac{\partial}{\partial t}\int_{V_0} W_0 dV + \int_{S_0} W dS = \int_{V_0} F dV, \tag{1}$$

$$\frac{\partial W_0}{\partial t} + divW = F. \tag{2}$$

Integral conservation laws (for example, mass, momentum, and energy for continuum models) are the most general form for describing the motion of media and are valid for both continuous and discontinuous solutions. Along with the integral, their differential form is used, which is valid only for continuous solutions. For example, the law of conservation of matter in gas dynamics is expressed by the continuity equation, for which the integral form has the form:

$$\frac{\partial}{\partial t}\int_{V_0} \rho dV + \int_{S_0} \rho \vec{v} dS = 0, \tag{3}$$

where ρ, v is the density and velocity vector of the liquid or gas. The differential form of the continuity equation is written as:

$$\frac{\partial \rho}{\partial t} + div\rho\vec{v} = 0. \tag{4}$$

Before modeling, it is necessary to determine what the ultimate goal of the study is, and what data is expected to be obtained as a result of solving the problem, what is the accuracy of the model, and with what accuracy is it necessary to obtain it. The decision what resources should be used in solving the problem and what opportunities (mathematical and technological). After analyzing the entire chain of process modeling processes, a conclusion is drawn about possible solutions to the problem based on existing models, numerical algorithms and technical means, or the conditions necessary for its solution are formulated (for example, requirements specification models, new algorithms are created, computational methods, etc.).

All classes of models for problems of mechanics can be divided into four levels:

1. Analytical approximations and linearized equations.
2. Equations without taking into account dissipative processes.
3. Equations taking into account dissipative processes.

4. Complete models described by equations that take into account real effects: the Navier-Stokes equation, taking into account compressibility and thermal conductivity, turbulence, etc. .. Equations of multicomponent and multiphase media, magnetohydrodynamic models, etc. [4].

The multi-parameter nature of the studied problems and the multi-scale processes, their non-linearity and multi-dimensionality do not allow us to formulate common approaches to the formulation of problems and obtaining solutions. The main types of development of mathematical modeling include the following areas:

- the use of models of different levels depending on the objectives of the study;
- the use of increasingly complex models that take into account a greater number of real physical effects of the investigated object;
- analysis of models, their systematization and identification of some classes of general models suitable for describing a wide range of tasks;
- further mathematical justification of physical and mathematical models and the correctness of the formulation of boundary-value problems [6].

Simplified models are obtained, as a rule, from higher-level models under various simplifying assumptions about the nature of the process under study. Thus, taking as a basis a more complete (covering) model, you can get a chain of simplified models. Using this approach allows reducing the number of models under consideration and focusing on the study of basic models describing entire classes of problems [7, 9].

The mathematical description of the process in heat exchangers is conveniently written in the form of an expression that characterizes the change in temperature in the heat carrier flow over time, due, firstly, to the movement of the flow and, secondly, to heat transfer.

If the structure of the coolant flow corresponds to the ideal mixing model, then for the mathematical description of this flow, you can use the equation taking into account the heat source that occurs in the flow due to heat transfer [1]:

$$Vc_\tau \frac{dT}{dt} = \upsilon c_\tau \left(T_{вх} - T\right) + Vq_\tau , \quad (5)$$

or

$$Vc_\tau \frac{dT}{dt} = \upsilon c_\tau \left(T_{вх} - T\right) + FK_\tau \Delta T, \quad (6)$$

where $Vc_\tau = FK_\tau\Delta T$ is the heat transfer intensity in the reaction volume V; q_τ is the specific volumetric intensity of the heat source; F is the heat transfer surface; K_τ – heat transfer coefficient; $\Delta T = (T_1\text{-}T_2)$ is the temperature difference between the primary and secondary coolants (the driving force of heat transfer).

If there is no mixing and the structure of the coolant flow corresponds to the ideal displacement model, then for the mathematical description of this flow, you can use the equation taking into account heat transfer:

$$s_B c_\tau \frac{\partial T}{\partial t} = -\upsilon c_\tau \frac{\partial T}{\partial t} + s_B q_\tau , \quad (7)$$

Since $V = s_B L$, where L is the length of the displacement zone, then

$$s_B q_\tau = \frac{s_B F K_\tau \Delta T}{s_B L} = \frac{F}{L} K_\tau \Delta T . \quad (8)$$

Then equation (7) can be rewritten as follows:

$$s_B c_\tau \frac{\partial T}{\partial t} = -\upsilon c_\tau \frac{\partial T}{\partial t} + \frac{F}{L} K_\tau \Delta T . \quad (9)$$

In equations (5) and (6), which are a mathematical description of the coolant flows in the ideal mixing and ideal displacement modes, respectively, taking into account heat transfer, it is assumed that the heat transfer coefficient of the QD through the wall separating the primary (“hot”) and secondary (“cold” ») Coolants, is a constant value that does not depend on their volumetric flow rates v_1 and v_2. Such an assumption simplifies mathematical calculations in solving optimization problems.

In cases where the dependence $K_T = f(v)$cannot be neglected, it is necessary to establish its nature and make a correction in the calculated expressions.

As examples of mathematical models of heat exchangers, the models of the simplest types of heat exchangers are analyzed below, in which heat is transferred between two flows – a heat carrier and a coolant. In all mathematical descriptions, it is assumed that the motion of the coolant and coolant flows is characterized by the simplest hydrodynamic models of “perfect mixing” and “perfect displacement”.

The nonlinearity of most of the problems under study does not allow us to obtain their exact solution. Moreover, such solutions do not always exist; therefore, the main methods for finding them are approximate and numerical. The former are based on some representation of a solution based on well-known assumptions about its nature. For example, in asymptotic methods in aerodynamics and combustion theory, the solution is presented in the form of an expansion in a small parameter. These approaches are applicable only for relatively simple tasks in which one type of flow predominates. Asymptotic methods are widely used at the initial stage of modeling; in each case, they require justification and analysis of the conditions of applicability of [7, 9].

The transition to more complex models required the development of numerical algorithms for solving multidimensional problems in the framework of various physical and mathematical models. At the present stage of development of mathematical modeling, the finite difference method, the finite volume method, the boundary element method, and a number of special techniques are widely used: the particle-in-cell method, the statistical test method, etc.

Mathematical modeling, along with physical and natural experiments, is the main way to study and acquire new knowledge in various fields of physics. It can be expected that in the future its role will increase, but it will not replace physical or natural experiments, since experience is always the basis of knowledge. It is possible rapprochement of various forms of study that complement each other.

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