Mathematical modeling of transfer processes and chemical reactions in catalytic membrane reactors
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Mathematical modeling of transfer processes and chemical reactions in catalytic membrane reactors

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Abstract

The aim of this work was investigation of mass transfer processes and chemical reactions proceeding in catalytic membrane reactors (CMR). These reactors are of great interest for chemical engineering since they enable to remove the equilibrium point to the side of forming the target products and enable to intensify the chemical processes. One of the perspective ways of using these reactors is getting hydrogen (for example by means of sulfur-iodine cycle).

Keywords: mathematical modeling; catalytic; membrane reactor; hydrogen; sulfur-iodine.

Hydrogen is used in chemical engineering mainly for production of HCl, NH_3, CH_3OH, organic substances. As hydrogen is absolutely harmless kind of fuel it could become the basis of hydrogen energetics. Really, the only product of hydrogen oxidation is water and nothing else. So, the possibility of using hydrogen as fuel is very attractive. That's why the problem of hydrogen production is a very important problem.

In this work the production of hydrogen was provided by means of using catalytic membrane reactor (CMR). This type of reactors is very perspective because of using the advantages of membrane division and catalysis. The principal scheme of CMR is shown on fig. 1. It looks like pipe heat exchanger. For the process of mathematical modeling its area was diversed into 4 zones: zone of outer space; zone of catalytic layer; zone of porous membrane; zone of internal space.

As a method of investigation of mass transfer processes and chemical reactions proceeding in catalytic membrane reactors the method of mathematical modeling was chosen. As the result of this modeling the time-dependent model with distributed parameters describing the processes proceeding inside the CMR was developed. For the forming of this mathematical model the block principle was used concerning the following: model structure of mathematical model, model of mass transfer processes and kinetic model of chemical reactions (Fig. 2).

For describing the processes inside the membrane of CMR the assumption that porous medium of the membrane is a nature fractal was used. This assumption gave us the possibility to consider the exponent of time derivative equel to fractional void volume.

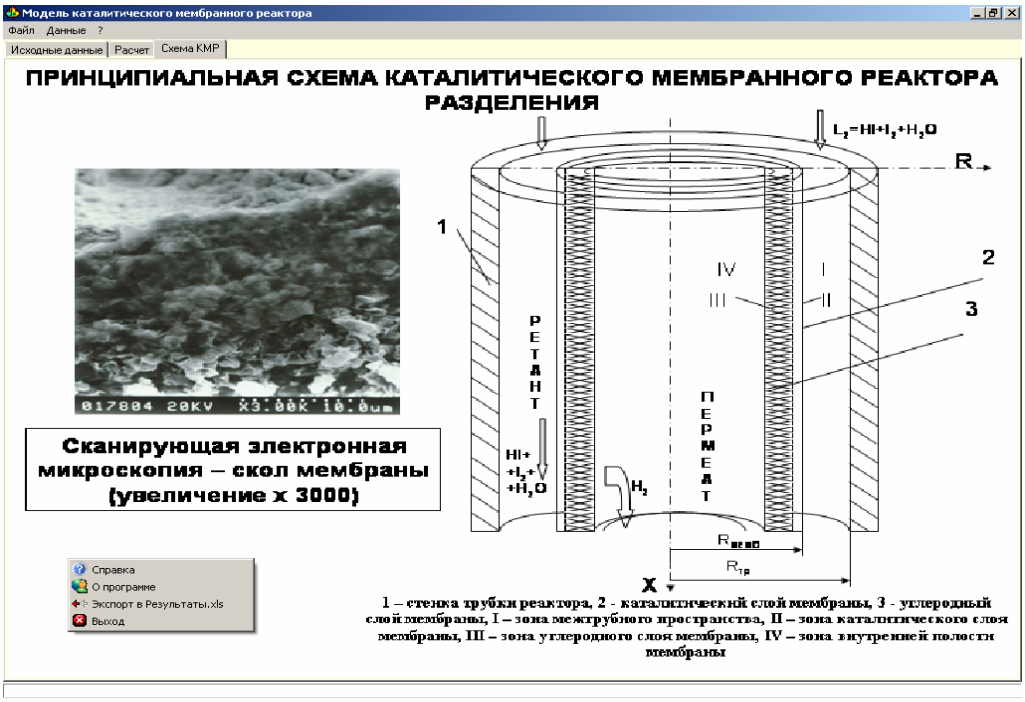

Fig. 1. Principal scheme of CMR

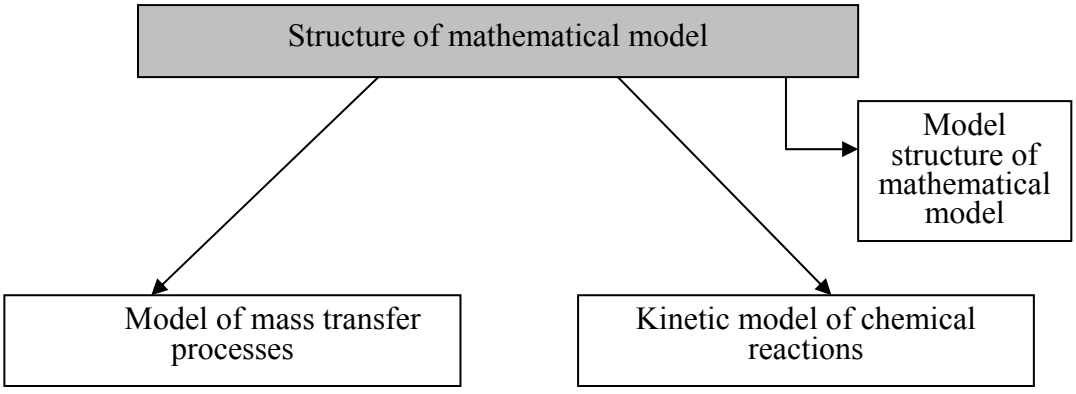

Fig. 2. Structure of mathematical model

Novation of this work consists in the fact that mathematical description of mass transfer processes is based on the usage of differential equations with time-derivative

of fractional order. The worked out mathematical model enables to determine (in the assumption of all starting value assignment) concentrations of all the components of the reactions in any place of the reactor at any moment of time. The model takes into account convective and diffusional mass transfer.

Main assumptions of the model are the following:

- The CMR works in isothermal conditions.
- Inside the 1-st and the 4-th zones the effective coefficients of diffusion in axial and radial directions are equal.
- Inside the 2-nd and the 3-rd zones there are no changes of component concentrations along the axial direction.
- Chemical reactions proceed only in the zone of catalytic layer.
- The kinetics of chemical reactions is described by law of interactive masses and the Arrenius equation.
- The structure of threads is described by means of the effective coefficients of diffusion.
- The threads of two adjacent zones are equal on the border of these zones.

Solving the equations of the model was carried out by means of the numerical methods of solving the equations of mathematical physics and chemistry based on the usage of the diversity schemes. The adequacy of exit data was estimated for the process of propane dehydration.

The above mentioned mathematical model of mass transfer processes and chemical reactions proceeding in catalytic membrane reactors was materialized by means of the worked out program product in order to simplify the processes of working with it and estimation of the results.

The worked out program product gives the possibility of exporting the results into the sheets of Microsoft Office Excel by means of using the DDE-technology of the application interaction. The integration of this program product into larger products by means of including the functions, procedures and the whole modules of the program product is also possible. The program includes the description and searh-information system, worked out by means of the utility Microsoft Help Workshop.

The graphical view of exit data of the program is shown on fig. 3. There we can see also the table view of this information.

The exit data of the worked out program product will be useful during the analysis of work of the CMR for the aim of determining for it optimal (concerning the chosen criterion) technological (temperature and pressure inside the CMR) and constructional (length of the apparatus, width of the catalyst layer, width of the mount) values.

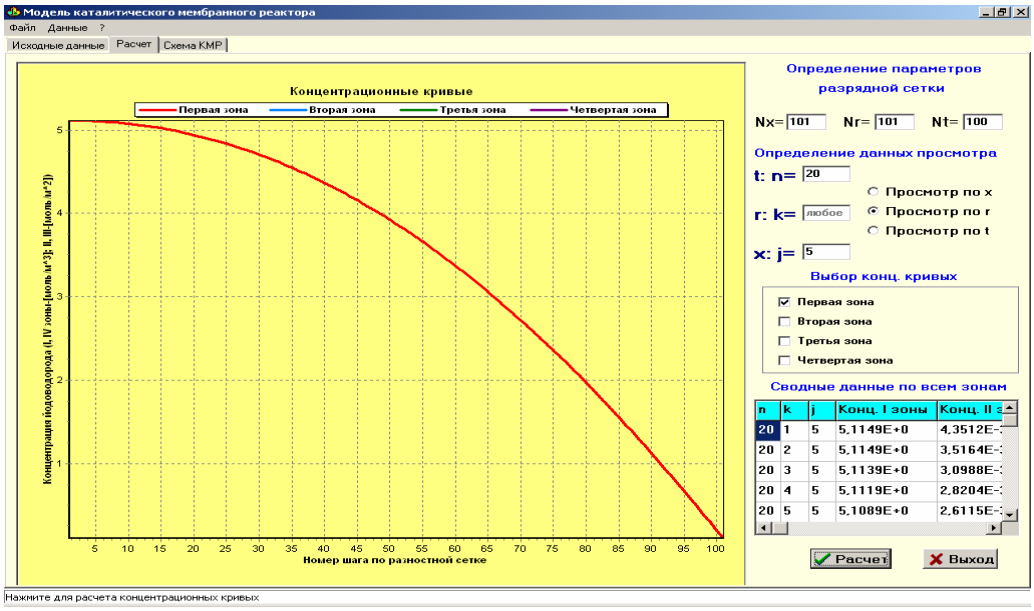

Fig. 3. Calculation tabsheet of the program Model_KMR_1

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