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Mathematical Modeling and Adaptive Algorithm for Calculating the Chemisorption Process in Regenerative Cartridge

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Abstract: The study presents a mathematical model describing mass transfer, thermal and hydro-mechanical processes in the regenerative cartridge with chemically bonded oxygen. The model takes into account the specifics of a gas mixture from the perspective of calculating its viscosity and thermal conductivity. The researcher propose an adaptive algorithm for solving the equations of the mathematical model with self-adjusting number of nodes of spatial sampling on the assumption of minimization of the integral criterion of accuracy.

Key words: Regenerative cartridge, mathematical model, adaptive algorithm, sorption process, thermal

INTRODUCTION

The challenge of protecting individuals or groups of people from exposure to external aggressive environment is not new. With the development of industry, science and technology the need for solving this problem has reached the level of economic and political significance. Therefore, research in the field of human protection is quite relevant (Putin, 2008).

One of the main classes of human technical protection systems are life support systems for physiological standards of respiration. Most of these systems are based on the principle of selective absorption of carbon dioxide from the exhaled gas mixture (Shumjackij, 2009).

A significant number of organizations around the world are engaged in the development and implementation of human protection systems using chemisorption process. As a rule, physical modeling is the main tool which is costly in terms of resources.

The development of information technology and the growth of computing capacities have made it possible to use the methods of mathematical modeling in solving a wide range of applications at various stages of the life cycle of human protection systems.

Availability of affordable computing capacities opens up new possibilities for research into high-performance algorithms to solve the equations of mathematical models that most accurately describe the character of mass transfer, thermal, hydrodynamic and chemical processes in the air recovery system. Currently, there are a lot of studies devoted to the development of highly adaptive algorithms for solving equations of mathematical models on computers. Mathematical models for regenerative cartridges with chemically bonded oxygen are no exception. The aim of this work is to develop an adaptive algorithm for solving the equations of mathematical models with self-adjusting parameters of a calculation scheme from the condition of minimization of the integral criterion.

MATERIALS AND METHODS

Mathematical modeling and development of adaptive algorithm for calculation: The process of chemisorption in the regenerative cartridge is represented as an object which receives at the input the flux characterized by the vector of input variables $u(\tau)$ which include composition and temperature of the input material flux, pressure, velocity, density, viscosity, etc. In the object, the input variables $u(\tau)$ undergo physical and chemical transformations into the variables $y(\tau)$ or in other words, the vector $u(\tau)$ under the action of some process operator is converted into a vector of output variables $y(\tau)$:

$$y(\tau) = T(u(\tau)) \quad (1)$$

In the general case, the operator reflects the totality of the simplest physical and chemical transformations occurring in the elements of the object and has a mixed deterministic-stochastic nature. The actual transformations Eq. 1 can be described by the mathematical model M, the equations of which can be solved using N algorithms:

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$$\tilde{y}_i(\tau) = M(A_i, u(\tau)), i = \overline{1, N} \quad (2)$$

in the form of a functional operator of input variables {u} into the estimation space of output variables $\{y_i\}$. Model Eq. 2 is an idealization of transformation Eq. 1 and reflects the degree of knowledge about the process. The vector of correct input variables y does not match the output of models given $\tilde{y}_i$ that the operator M is an approximate characteristic of T and is determined by the features of the calculation algorithm A_i. An essential feature of the identity of the operators T and M is the proximity of functions $\tilde{y}_i(\tau)$ and $y(\tau)$ from the viewpoint of a particular norm $R(y(\tau), \tilde{y}_i(\tau))$.

In the explicit form the operator performing the transformation Eq. 2 is a closed system of equations and different ratios of empirical character supplemented with the necessary initial and boundary conditions. The choice of algorithm is the process of adapting the calculation scheme.

Thus, the solution of the problem of constructing an adaptive algorithm for calculating the equations of the mathematical model with self-adjusting parameters of the calculation scheme from the condition of minimizing the integral criterion is to form a plurality of algorithms for calculating and selecting the algorithm Δ_i that provides the proximity of functions $\tilde{y}_i(\tau)$ and $y(\tau)$ from the viewpoint of a particular norm $R(y(\tau), \tilde{y}_i(\tau))$.

We consider the generalized scheme of the sorption process in the regenerative cartridge shown in Fig. 1. The sorption layer is presented in the form of a cylinder of length L and the flux section area S. The input of the sorption layer (x = 0) receives the gas mixture at a rate G and pressure P_{in}, temperature T_{in} and composition $c_{in} = \{c_{1, in}, c_{2, in..}, c_{n, in}\}$. As the gas mixture passes through the granular layer, the selective sorbent adsorption of carbon dioxide and release of oxygen occur. At the output of the sorption layer, we get a gas mixture at a rate of G, the pressure P_{out}, temperature T_{out} and composition $c_{out} = \{c_{1, out}, c_{2, out}, ..., c_{n, out}\}$.

In the mathematical description of the processes in regenerative cartridge we arrange the coordinate axis O_z along the path of the gas mixture as shown in Fig. 1 and take the following assumptions:

- Gas mixture is an ideal gas
- Thermophysical properties of the sorbent granules are constant in time
- Thermal effect of sorption is constant
- Heat capacity of gas mixture does not depend on temperature but it depends on the composition
- Velocity of gas mixture is constant along the length of the granular sorbent bed
- There are no thermal losses into the environment
- Gas mixture consists of n components (1-carbon dioxide, 2-oxygen, 3-nitrogen)

According to the accepted assumptions, the mathematical model takes the form Khajuria (2011), Agarwal (2010), Yavary *et al.* (2015) and Dang *et al.* (2013). Equations of componentwise material balance:

$$\varepsilon\frac{\partial c_i}{\partial \tau} + v\frac{\partial c_i}{\partial z} + \rho_a\frac{\partial a_i}{\partial \tau} = D_{z,i}\frac{\partial^2 c_i}{\partial z^2}, i = \overline{1, n} \quad (3)$$

Where:

ε = Porosity of the adsorbent layer
c_i = Concentration of the ith component of gas mixture (mol/m^3)
τ = Time (c)
v = Velocity of gas mixture along the axis Oz (m/sec)
z = Vertical coordinate (m)
ρ_a = Bulk density of adsorbent granules (kg/m^3)
a_i = The value of sorption of the ith component, (mol/kg)
$D_{z,1}$ = Diffusion coefficient of the ith component along the axis Oz (m^2/sec)
n = The number of gas mixture components

Trepnel's kinetic equations:

$$\frac{\partial a_i}{\partial \tau} = \beta_i\frac{c_i}{\rho_a}\left[1 - \frac{a_i}{a_{i_0}}\right]^2, \quad i = \overline{1, n} \quad (4)$$

Where:

β_i = Kinetic coefficients for the ith component 1/s
a_{i0} = Ultimate capacity the sorbent for the ith component (mol/kg)

The equation of thermal balance for sorbent granules:

$$\rho_a\gamma_a\frac{\partial T_a}{\partial \tau} = -\rho_a\sum_{i=1}^{n}\Delta H_i\frac{\partial a_i}{\partial \tau} + \lambda_a\frac{\partial^2 T_a}{\partial z^2} + Kf(T - T_a) \quad (5)$$

Where:

γ_a = Specific heat capacity of the sorbent (J/(kg K))
ΔH_i = Thermal effect of sorption for the ith component (J/mol)
λ_a = Sorbent thermal conductivity coefficient (W/(mK))
K = Heat transfer coefficient from the granular layer to the gas mixture (W/(m^2 K))
f = Specific surface area of Sorbent particles (m^2/m^3)
T = Gas mixture temperature (K)
T_a = Sorbent granules temperature (K)

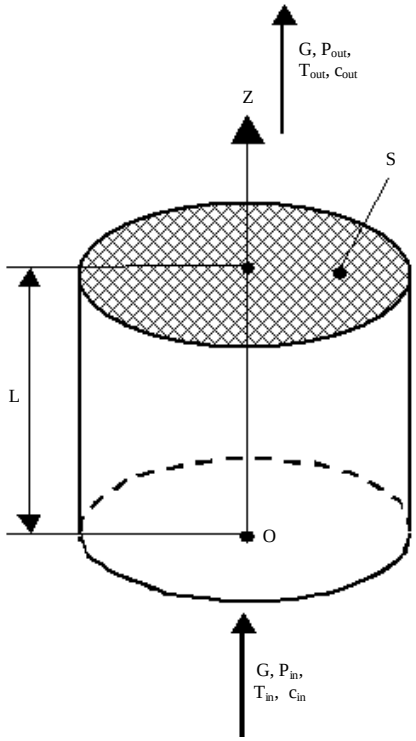

Fig. 1: The scheme of the sorption process in the regenerative cartridge

The equation of thermal balance for gas mixture:

$$\varepsilon\rho\gamma\frac{\partial T}{\partial \tau} = \gamma v\rho\frac{\partial T}{\partial z} - p\frac{\partial v}{\partial z} + \varepsilon\lambda\frac{\partial^2 T}{\partial z^2} - Kf(T - T_a) \quad (6)$$

Where:

γ = Specific heat capacity of gas mixture (J/(mol K))
T = Gas mixture temperature (K)
P = Gas mixture pressure (Pa)
λ = Thermal conductivity coefficient of gas mixture (W/(m K))

The Kozeny-Carman equation of momentum conservation:

$$v = -\frac{d^2\varepsilon^3}{150(1-\varepsilon)^2\mu}\frac{\partial P}{\partial z} \quad (7)$$

Where:

d = Diameter of granules of sorbent particles (m)
μ = Coefficient of dynamic viscosity of gas mixture (Pa)

The equation of the total mass balance of gas phase:

$$\rho = \sum_{i=1}^{n} c_i \quad (8)$$

The equation of of state of ideal gas:

$$P = \rho RT \quad (9)$$

Equations of concentration constraints:

$$y_i = \frac{c_i}{\rho}, i = \overline{1, n} \quad (10)$$

where, y_i is relative concentration of the ith component of gas mixture (mol/mol). Models of physical properties of gas mixture; molar mass of gas mixture M:

$$M = \sum_{i=1}^{n} M_i y_i \quad (11)$$

where, M_i is molar mass of the ith component of gas mixture kg/mol. Thermal conductivity coefficient of gas mixture λ (Brokaw method) (Ried *et al*., 1987):

$$\lambda = k\sum_{i=1}^{n}\lambda_i y_i + \frac{1-k}{\sum_{i=1}^{n}\frac{y_i}{\lambda_i}}$$
$$\lambda_i = \lambda_{i,0} + \Delta\lambda_{i,1}(T - 273,15)\ i = \overline{1, n} \quad (12)$$

Where:

k = Experimental coefficient selected based on the specifics of gas mixture
λ_i = Thermal conductivity coefficient of the ith component of gas mixture (W/(m K))
$\lambda_{i,0}$ = Thermal conductivity coefficient of the ith component of gas mixture at 0°C (W(m K))
$\Delta\lambda_{i,1}$ = Variation of the thermal conductivity of the ith component of gas mixture at the temperature change of 1°C (W/(m K^2))

Specific heat capacity of gas mixture:

$$\gamma = \sum_{i=1}^{n}\gamma_i y_i \quad (13)$$

where, λ_i is specific heat capacity of the ith component of gas mixture (J/(kg K)). Dynamic viscosity coefficient of gas mixture is calculated by Herning and Zipperer's method (Ried *et al*., 1987; Bogoslovskij, 2001):

$$\mu = \sum_{i=1}^{n}\frac{\mu_i y_i}{\sum_{i=1}^{n} y_i\sqrt{\frac{M_i}{M_j}}}, \mu_i = \mu_{i,0} + \Delta\mu_{i,1}(T - 273,15), i = \overline{1, n} \quad (14)$$

Where:

μ_i = Dynamic viscosity coefficient of the ith component of gas mixture (Pa s)

$\mu_{i,0}$ = Dynamic viscosity coefficient of the ith component of gas mixture at 0°C (Pa sec)

$\Delta\mu_{i,1}$ = Variation of dynamic viscosity coefficient of the ith component of gas mixture at temperature change of 1°C ((Pa sec)/K)

Initial conditions:

$$T(z, 0) = T_0(z),\ T_a(z, 0) = T_{a_0}(z)$$
$$c_i(z, 0) = c_{i_0}(z),\ a_i(z, 0) = a_{i_0}(z),\ i = \overline{1, n} \quad (15)$$

where, $T_0(z)$, $T_{a0}(z)$, $c_{i0}(z)$, $a_{i0}(z)$ is distribution of model variables in the coordinate z at the initial time. Boundary conditions at the input (z = 0):

$$D_{z,i}\frac{\partial c_i(0,\tau)}{\partial z} = \frac{G}{S}(c_i(0,\tau)-c_{i,in}(\tau)),T(0,\tau) = T_{in}(\tau)$$
$$\frac{\partial T_a(0,\tau)}{\partial z} = \lambda(T_a(0,\tau)-T_{in}(\tau)) \quad (16)$$

Boundary conditions at the output (z = L):

$$\frac{\partial c_i(L,\tau)}{\partial \tau} = 0, \frac{\partial T(L,\tau)}{\partial z} = 0, \frac{\partial T_a(L,\tau)}{\partial z} = 0 \quad (17)$$

Thus, Eq. 3-17 are a mathematical description of mass transfer, thermal and hydrodynamic processes in the regenerative cartridge with chemically bonded oxygen. To calculate the equations of mathematical model of the regenerative cartridge we used the method of straight lines (Hairer *et al*., 1996). The system of equations was sampled with respect to variable z, there by turning it into a system of ordinary differential and algebraic equations, for the integration of which we used the Runge-Kutta method with automatic step selection. The main advantage of the method of straight lines is that the spatial sampling can be performed with a high density of nodes and that there is an integration error checking mechanism and thus, a high accuracy of approximation of solutions both in time and in the coordinate z can be achieved. In accordance with the method of straight lines in the mathematical model Eq. 3-17 the derivatives are approximated by z finite differences (Table 1):

$$\frac{\partial F_i(z,\tau)}{\partial z} = \frac{k_1F_{i+2}+k_2F_{i+1}+k_3F_i+k_4F_{i-1}+k_5F_{i-2}+k_6F_{i-3}}{k_0h_z} \quad (18)$$

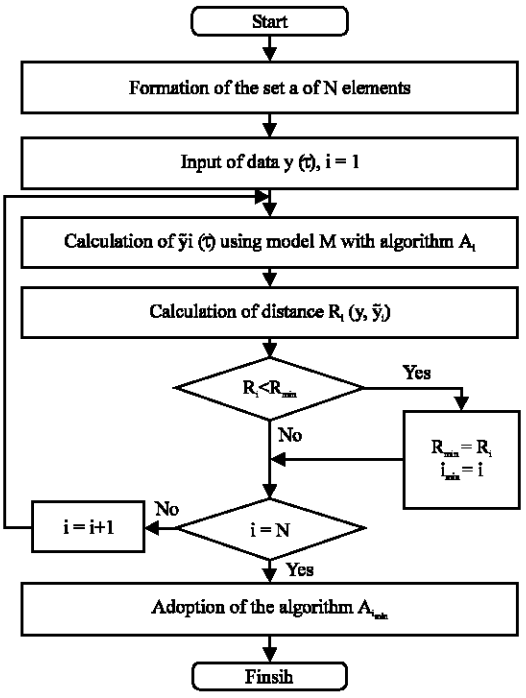

Fig. 2: A block diagram of the adaptation process of the calculation scheme

Table 1: Possible options for approximation of the first derivative

N_2	k_0	k_1	k_2	k_3	k_4	k_5	k_6
1	1	0	0	1	-1	0	0
2	2	0	0	3	-4	1	0
3	2	0	1	0	-1	0	0
4	12	-1	8	0	-8	1	0
5	6	0	2	3	-6	1	0
6	8	0	3	3	-7	1	0
7	12	0	3	7	-11	1	0
8	12	0	3	10	-18	6	-1
9	1	0	0.25	0.75	-1.25	0.25	0

$$\frac{\partial^2 F_i(z,\tau)}{\partial z^2} = \frac{F_{i+1} - 2F_i + F_{i-1}}{h_z^2} \quad (19)$$

Where:

$F_i(z, \tau)$ = The value of model variable in the ith node of spatial sampling

k_i = Weighting factors of difference scheme

h_2 = Step sampling along the axis Oz

Figure 2 is a block diagram of the calculation scheme adaptation of mathematical model equations for the processes in the regenerative cartridge. The algorithm begins with a process of forming a set from N algorithms. The general view of the approximation of a derivative of the 1st order is represented by Eq. 16. Various N sets of values of weighting coefficients k allow generating a set

of N algorithms. Table 1 shows the possible sets of weighting coefficients for N = 9 algorithms (Korn and Korn, 2000).

The next step of the algorithm introduced the initial pilot (reference) data. Measurement data of output curves $c_i(L, \tau)$ are most commonly used as experimental data of chemisorption cartridges. Further, evaluation of A_i, algorithm is calculation of the quality score of R_i of the form:

$$R_i = \int_0^{\tau} (y(\tau) - \tilde{y}_i(\tau))^2 d\tau \quad (18)$$

where, τ_k is the end time of the process of observation (s). The next step is a comparison of the value of R_i criterion with a minimum value R_{min} which was recorded in the previous steps or set in advance. If R_i is less than R_{min}, the value of R_i and the number of the corresponding algorithm i_{min} are stored as a new value of the criterion. In the following step we check the current index i. If its value is equal to the number of N algorithms, the enumeration process ends and Ai_{min} is adopted as the algorithm, otherwise we proceed to the next A_{i+1} algorithm.

RESULTS AND DISCUSSION

Figure 3 shows the results of calculation of the carbon dioxide output curves for a variety of approximations of the first derivative where a triangle marks the experimental values of the output concentration of carbon dioxide in the regenerative cartridge. The number of the algorithm is specified in the curve as shown in Table 1. Thus, the minimum value of the integral Eq. 20 was obtained for the difference scheme 8 and amounted to $R_{min} = R_8 = 57.78$.

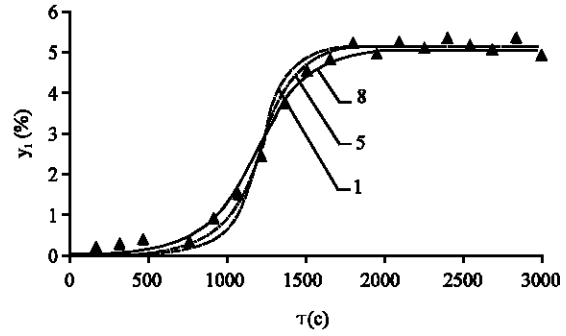

Fig. 3: The results of the calculation of output curves for carbon dioxide

CONCLUSION

As expected in the case of the sorption front blurring the most accurate difference schemes are those that use the largest number of sampling nodes. However, for "extreme" sorption fronts the most appropriate schemes are those with the least amount of sampling points. In the case of the oscillation curves, it is necessary to supplement the set of algorithms with flux limited difference schemes (Harten and Osher, 1987).

Thus, the proposed approach is an adaptive algorithm for solving the equations of mathematical model with self-adjusting parameters of the calculation scheme from the condition of the minimization integral criterion.

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