ISSN: 2350-0328

International Journal of Advanced Research in Science, Engineering and Technology

Vol. 6, Issue 10 , October 2019

Algorithm for Determining Unmeasured Coordinates During the Absorption of Ammoniated Brine

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ABSTRACT: The article considers the creation of an algorithm for determining the unmeasured coordinates of an object that has a complex structure. The features of constructing a mathematical model of the absorption process upon receipt of the ammoniated brine are given. The mathematical dependence of the measured coordinates are determined. A method is proposed for reconstructing immeasurable variables based on measured input and output coordinates. A recommendation is given to determine the number of equations, which are the number of necessary unmeasured variables for the preparation of the equation of state. A systematic approach to the development of mathematical models, taking into account the reversibility of the ongoing reactions, as well as the possibility of recovering unmeasurable from the measured, is proposed. It allows the development of high-quality process control systems. The rationale of the model structure for the operational management of a wide class of objects of chemical processes of synthesis with reversible reactions is substantiated. Algorithms have been developed to determine the unmeasured output coordinates of the system and external disturbances during the operation of the system.

KEY WORDS: unmeasured coordinates, steps of discreteness, matrix, dynamical system, ammoniated brine, algorithms, reversible reactions.

I.INTRODUCTION

One of the most characteristic features of modern chemical and food industries is the desire to improve technologies, increase equipment productivity and increase the capacity of technological production units. Moreover, the development of modern production is accompanied by a continuous increase in the requirements for the quality of functioning of technical systems, which must be taken into account at the stage of development of process control systems. Organization of modern production management requires a revision of traditional control schemes and a new systems approach to the development of automation systems. In this case, it is necessary to consider the objects under study as a single technical system, which includes all control devices and takes into account the interconnection and influence of these devices on each other.

The process under consideration for the production of ammoniated brine can be characterized as a multi-stage process with a large number of reversible reactions. The input variables are weak ammoniated brine, gaseous ammonia, and the output variables are hot ammoniated brine, exhaust absorption gas. Each of the technological flows is characterized by a set of information variables, which at this stage of modeling are proposed to be divided into four classes:

- parameters whose operational measurement is possible;
-parameters, which cannot be measured promptly;
- parameters that are entered by the operator (laboratory analysis data or coefficients for tuning, training the model in real time);
- design parameters, the operational measurement of which is possible.

Under such circumstances, the creation or improvement of the existing absorption process control system is directly related to the development of mathematical models for conducting a simulation experiment.

II. METHODOLOGY

In mathematical modeling of chemical-technological dynamic systems, it is necessary, first of all, to choose the coordinates in which the dynamic system will be considered. For example, depending on the choice of space, a

ISSN: 2350-0328

International Journal of Advanced Research in Science, Engineering and Technology

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stationary process can be expressed by a point or a set of trajectories, the position of which does not depend on time. The latter is due to the fact that when compiling a system of differential equations, the parameter t can be either physical time, or any analogue of it. For example, as such a parameter f in an absorption column, one can consider the residence time in the absorber; h column height.

The model of continuous absorption of a multicomponent mixture, where the physicochemical process takes place, is:

$$\frac{d\bar{x}}{dh} = \frac{A}{L}(B)\left[\overline{(y^* - x^*) - (y - x)}\right] \quad (1)$$

Here (B) - is the square symmetric matrix of mass transfer coefficients with a positive determinant; A - hydrodynamic factor, equal to dF/dh, where F is the mass transfer surface, h - is the height of the column; L - the number of moles of the liquid phase stream per unit time; $y^* - x^*$ - node liquid-vapor thermodynamic equilibrium; $y - x$ - a working node that combines the compositions of the liquid and vapor flow in each section of the column in which the differential absorption process takes place.

The working node is obtained using the balance equation of the column section:

$$\overline{y - x} = (1 - m_i)(x^k - x), \quad (2)$$

where m_i is the ratio of the liquid (L) and vapor (V) flows in the sections: $m_i = \frac{L}{V}$ for the strengthening section, for the exhaust section $m_i = (L + F)/V$, F - the amount of the initial mixture when it is supplied as liquid, x^k is the composition of the final product of the absorber (ammoniated brine).

Mathematical modeling of chemical reactions having a complex mechanism of flow through several intermediates is a rather laborious task, usually solved only with the help of computers [24, 25]. Even the use of dimensionless quantities, which makes it possible to represent a dynamic system on a plane, does not always significantly simplify the task.

It should be noted that this mathematical model uses only those parameters that can be directly measured. The second part of the mathematical model is based on virtual parameters, i.e. information decomposition results.

In the process of functioning of the system in real conditions, it is impossible to measure some parameters that significantly affect the quality of control. Therefore, when creating highly efficient control systems, it becomes necessary to restore the values of these unmeasured coordinates.

Consider the question of determining unmeasured coordinates during the operation of the system. Let the differential equations of the object be given, external disturbances and a sequence of control vectors are known. Measured using sensors $m>n$ coordinates of the output vector of the system. It is required to find an algorithm for determining (for a certain minimum number of steps of discreteness) a sequence of unmeasured coordinates of the output vector. First we find the necessary initial number of steps of discreteness k_{sd} .

We write the system of equations of state parameters for $k = ,1,2,3\ldots, k_{sd}$:

$$y[T] = W(T)\{y[0] + A_1(T)u[0] + C_1(T)\,f[0]\};$$

$$y[2T] = W(T)\{y[T] + A_1(T)u[T] + C_1(T)\,f[T]\};$$

……...

$$y[k_{sd}T] = W(T)\{y[(k_{sd} - 1)T] + A_1(T)u[(k_{sd} - 1)T] + C_1(T)\,f[(k_{sd} - 1)T]\}.$$

The system of equations contains the known matrices $W(T), A_1(T), C_1(T)$ and the known sequences $u(kT)$ and $f(kT)$.

We divide the output vector of the system $y(kT)$ into two vectors: the vector of measured output coordinates $y_m[kT]$, which includes all m coordinates measured by sensors, and the vector of unmeasured coordinates $y_{um}[kT]$, which includes all other $n - m$ coordinates. In the first equation of the system, the number of unknown output

ISSN: 2350-0328
International Journal of Advanced Research in Science, Engineering and Technology
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coordinates is $2(n-m)$. In all subsequent $(k_{sd}-1)$ equations, the number of unknown coordinates is $(k_{sd}-1)(n-m)$.

Thus, the total number of unknowns will be determined by the formula:

$$g=(k_{sd}-1)(n-m)$$

The number of equations for their determination is n, and a certain number of equations $g_0<n$ may be superfluous. The required number of steps of discreteness for determining g unknowns is determined from the equality

$$k_{sd}-g_0=(k_{sd}+1)(n-m)$$

Whence $$k_{sd}=\frac{n-m+g_0}{m}.$$

To determine the required number of steps of discreteness, you can also use the formula

$$k_{sd}\geq\frac{n-m}{m}.$$

If the number is fractional $\frac{n-m}{m}$, then the nearest large integer is taken k_{sd}. The number of unnecessary equations is calculated by the formula:

$$g_0=(k_{sd}+1)n-m$$

After the initial number k_{sd} at each step, the number of unknowns for the next step will always be less than the number of equations that can be used to determine them, since $m<n$. Therefore, only for the initial number of steps $k_{sd}\geq 1$. We find formulas for calculating uncountable coordinates. Transforming the system of equations, we obtain:

$$\begin{gathered} y[T]-H(T)u[0]-G(T)f[0]=W(T)y[0]; \\ y[2T]-H(T)u[T]-G(T)f[T]=W(T)y[T]; \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \\ y[k_{sd}T]-H(T)u[(k_{sd}-1)T]-G(T)f[(k_{sd}-1)T]=W(T)y[(k_{sd}-1)T]. \end{gathered} \quad (3)$$

We introduce into the considered submatrices $W_u(T)$ and $W_n(T)$, which are obtained from the matrix $W(T)$ according to the following rule. The submatrix $W_u(T)$ is obtained from the matrix $W(T)$ by eliminating all j-columns that correspond to the numbers of unmeasured coordinates. Excluded columns make up the shortened matrix $W_n(T)$. So the expression:

$$W(T)y[kT]$$

taking into account the separation of the vector $y[kT]$ into two vectors, we can write this:

$$W(T)y[kT]=W_u(T)y_u[kT]+W_H(T)y[kT] \quad (4)$$

We will perform a similar operation for the identity matrix E of type $n\times n$ and we will have

$$Ey[kT]=E_U y_U[kT]+E_H y_H[kT] \quad (5)$$

Given formulas (4) and (5), we obtain the expression for the k-th equation of the system in the following form:

$$\begin{gathered} E_U y_U[(k+1)T]-W_U(T)y_U[kT]-H(T)u[kT]-G(T)f[kT]= \\ =W_H(T)y_H[kT]-E_H y_H[(k+1)T] \end{gathered}$$

By combining the coordinates of the vectors $y_H[kT]$ and $y_H[(k+1)T]$ into one vector

$$y_H^k=(y_H[kT],y_H[(k+1)T])^T,$$

we get $E_U y_U[(k+1)T]-W_U y_U[kT]-H(T)u[kT]-G(T)f[kT]=L_K y_H^k$, (6)

ISSN: 2350-0328
International Journal of Advanced Research in Science, Engineering and Technology
Vol. 6, Issue 10 , October 2019

$(k = 0,1,2,3...k_{sd} - 1)$

where L_k denotes a matrix consisting of two cell matrices:

$$L_k = (W_H(T) - E_H)$$

The set of equations (6) can be written as follows:

$$\theta_0 = L_{H0} y_H$$

where $\theta_0 = \begin{Vmatrix} E_U y_U[T] - W_U y_U[0] - H(T)u[0] - G(T) f[0] \\ E_U y_U[2T] - W_U y_U[T] - H(T)u[T] - G(T) f[T] \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ E_U y_U[k_{sd}T] - W_U y_U[(k_{sd}) - T] - H(T)u[(k_{sd}) - T] - G(T) f[(k_{sd}) - T] \end{Vmatrix}$

and $L_{H0} = \begin{Vmatrix} W_H & -E_H & 0 & \ldots & 0 & 0 \\ 0 & W_H(T) & -E_H & \ldots & 0 & 0 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \\ 0 & 0 & 0 & \ldots & W_H(T) & -E_H \end{Vmatrix}$,

$$y_H = \left(y_H[0] y_H[T] .. y_H[(k_{sd} - 1)T]\right)^T$$

If $g_0 \neq 0$, then the extra number of rows of the matrices θ_0 and L_{H0} the system, numerically equal to the value g_0, is excluded in such a way that the rank of the matrix L_H, which is obtained after excluding the rows, is equal to the number of unknown unknowns. Get a new system

$$\theta = L_H y_H,$$

where θ and L_H are the vector and matrix, respectively, resulting from the exclusion g_0 of rows. We write the solution of the system in the form

$$y_H = L_H^{-1}\theta.$$

The equation of state parameters for subsequent steps of discreteness will have the form

$$y[(k_{sd} + i)T] = W(T) y[(k_{sd} + i - 1)T] + H(T)u[(k_{sd} + i - 1)T] + G(T) f[(k_{sd} + i - 1)T]$$
$$(i = 1,2,3,\ldots). \quad (8)$$

Given formula (7), after the transformations, we obtain

$$E_H y_H[(k_{sd} + i)T] = W(T) y[(k_{sd} + i - 1)T] - E_U y_U(T) +$$
$$+ H(T)u[(k_{sd} + i - 1)T] + G(T) f[(k_{sd} + i - 1)T]$$

From the system of equations (8), we exclude those rows in which the matrix F_H contains zeros, then we obtain a recurrent system of equations for calculating the unchanged coordinates:

$$y_H[(k_{sd} + i)T] = W_y(T) y[(k_{sd} + i - 1)T] + H_y(T)u[(k_{sd} + i - 1)T] +$$
$$+ G_y(T) f[(k_{sd} + i - 1)T] \qquad (i = 1,2,3,\ldots), \quad (9)$$

where $W_y(T), H_y(T), u\ G_y(T)$ the truncated matrices are denoted by. They are obtained by excluding those rows of matrices $W(T), H(T) and\ G(T)$ that correspond to zero rows of the matrix E_H.

III. RESULTS

Using this mathematical model as part of the absorption process control system will allow:

ISSN: 2350-0328

International Journal of Advanced Research in Science, Engineering and Technology

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-reduce the loss of ammonia gas;
-increase the production yield of the target product-soda ash;
- to improve the quality of the obtained ammoniated brine by reducing the content of products of side redox processes.

IV. CONCLUSION

The proposed systematic approach to the development of mathematical models that take into account the reversibility of ongoing reactions, as well as the possibility of recovering unchanged from the measured ones, allows developing high-quality process control systems.
The conducted studies made it possible to substantiate the rationality of the structure of the model for the operational management of a wide class of objects of chemical processes of synthesis with reversible reactions.
Thus, as a result of the above analysis, algorithms were found to determine the unmeasured output coordinates of the system and external disturbances during the operation of the system. The required minimum initial number of steps (8), and the algorithm for determining the generalized vector is given by formula (9).

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