VII International Scientific Practical Conference "Innovative Technologies in Engineering" IOP Publishing
IOP Conf. Series: Materials Science and Engineering **142** (2016) 012033 doi:10.1088/1757-899X/142/1/012033

Mathematical Modeling of Non-Stationary Hydraulic Process Occurring in the Gas Centrifuge Cascade During the Separation of Multicomponent Isotope Mixtures

A A Orlov[1], A A Ushakov[2] and V P Sovach[2]

[1] National Research Tomsk Polytechnic University, 634050, Lenin av, 30, Tomsk, Russia
[2] SC "PA Electrochemical Plant", 663690, Pervaya promyshlennaya ul, 1, Zelenogorsk, Russia

E-mail: ushakovaa2015@sibmail.com

Abstract. This article presents results of development of the mathematical model of nonstationary separation processes occurring in gas centrifuge cascades for separation of multicomponent isotope mixtures. This model was used for the calculation parameters of gas centrifuge cascade for separation of germanium isotopes. Comparison of obtained values with results of other authors revealed that developed mathematical model is adequate to describe nonstationary separation processes in gas centrifuge cascades for separation of multicomponent isotope mixtures.

1. Introduction

Gas centrifuge (GC) method of isotope separation is industrial method of uranium enrichment. High efficiency and long-term experience of gas centrifuge operation enabled to extend the application domain of this separation method and devise the industrial plant for separation stable and radioactive isotopes of various chemical elements.

Process gases are used for isotope separation by GC method. The molecules of this gases consists of the atoms of one or several chemical elements (for example, Kr, Xe, SiF_4, WF_6, $Fe(CO)_5$, $Cd(CH_3)_2$). Therefore, process gas is called a multicomponent isotope mixture (MCIM).

Technological processes of MCIM separation in GC cascade goes continuously in the stationary mode. In the operation of cascade there are nonstationary hydraulic processes, characterized by time-variable values of MCIM pressure and flows in cascade stages. For example a filling of GC cascade by process gas is nonstationary hydraulic process.

During nonstationary processes it is necessary to ensure safety of the equipment and to minimize losses of cascade productivity. The GC cascades for MCIM separation have insignificant gas content, and, as a consequence, low inertia. It leads to increased influence of nonstationary processes on the cascade efficiency.

In this regard, actual task is full-scale research of nonstationary process.

This problem had been discussed in the papers [1-7], authors of which had developed of dynamic stability principles, analytical and numerical solution methods of nonstationary hydraulic equations and mathematical models of nonstationary processes in free cascades. These processes was researched in the cascades for uranium isotopes separation. The presented models have different object details.

In paper [2] there was the description of the nonstationarity's influence during multicomponent isotope mixture separation processes. The papers about developed mathematical models of nonstationary hydraulic processes in these cascades don't exist.

We have developed of mathematical model of nonstationary hydraulic processes in gas centrifuge cascade for separation of multicomponent isotope mixtures and realized it as program software.

2. The description of mathematical model of nonstationary processes

2.1. Basic parameters of stage and cascade

MCIM separation takes place into a cascade (figure 1). A cascade consists of S separation stages numbered by i index ($i=\overline{1,S}$) and connected by counter-current type [1]. The cascade has three flows: incoming feed flow F, output light fraction flow P and heavy fraction flow W.

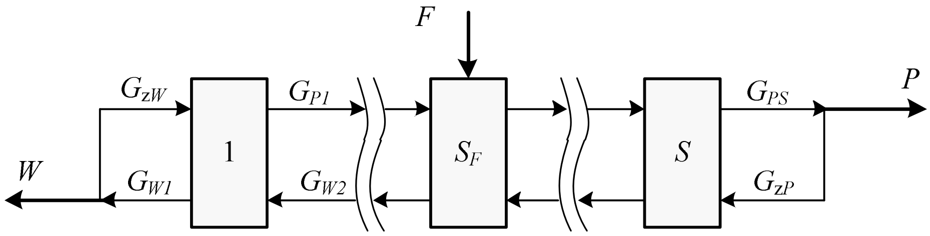

Figure 1. Separation cascade.

Separation stage consists of n parallel-connected GC. The stage has three flows: incoming feed flow G_F, output light fraction flow G_P and heavy fraction flow G_W (figure 2).

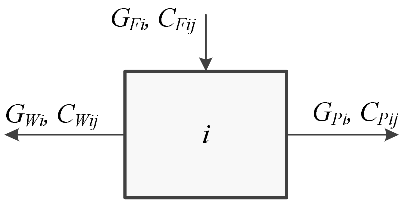

Figure 2. Separation stage.

During stationary hydraulic process the flows and concentrations of components in stage are interrelated by material balance equations and balance equations of each component (in the absence of material losses):

$$G_{Fi} = G_{Pi} + G_{Wi}\,, \tag{1}$$

$$\theta_i = \frac{G_{Pi}}{G_{Fi}}, \tag{2}$$

where θ_i is cut of the *i*-th stage.

The flows of cascade and concentrations of the components are interrelated by balance equations:

$$F = P + W. \tag{3}$$

1.2. Capacities of model

A method of calculation non-stationary separation processes is based on the following points:

1. Each stage is composed of finite number of capacities. The value of process gas into cascade (the holdup) is distributed in these capacities.
2. The condition of process gas into capacity is characterized by pressure value.
3. Basic equation of mathematical model is balance equation of process gas and some components in each capacity.

Each capacity has the following properties: the volume V; the pressure of process gas P, concentration of the j-th component C_j, physical properties of process gas (molar mass μ, dynamic viscosity η, the temperature T); the quantity of process gas into capacity (holdup) H.

In the regards, the holdup of cascade is distributed in 4S capacities: feed manifold, GC, heavy fraction manifold and light fraction manifold (figure 3).

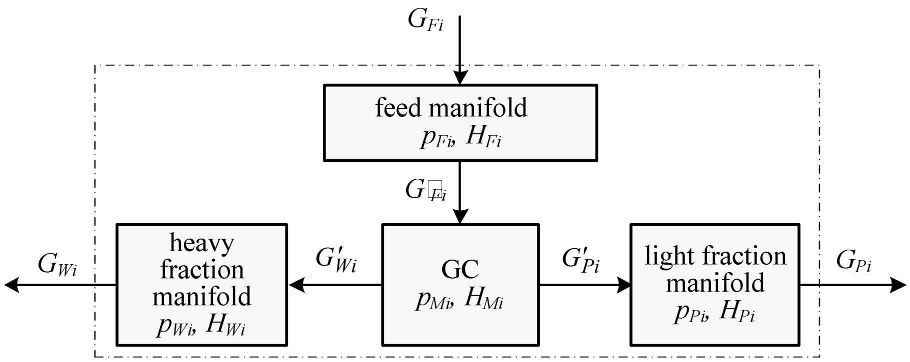

Figure 3. Capacities of *i*-th stage.

The incoming flow G_{Fi} enters to feed manifold. The flow G'_{Fi} comes in GC and have been separated to flows G'_{Pi} and G'_{Wi} which left to light fraction manifold and heavy fraction manifold. The flows G_{Pi} and G_{Wi} left out from the stage.

The value of concentration C_{Fij} is given by:

$$C_{Fij} = \frac{1}{G_{Fi}} \cdot \begin{cases} \delta_i F C_{Fj} + G_{zW} C_{Wij} + G_{Wi+1} C_{Wi+1j}, & i = 1 \\ \delta_i F C_{Fj} + G_{Pi-1} C_{Pi-1j} + G_{Wi+1} C_{Wi+1j}, & i = \overline{2; S-1} \\ \delta_i F C_{Fj} + G_{Pi-1} C_{Pi-1j} + G_{zP} C_{Pij}, & i = S \end{cases}, \tag{4}$$

$$\delta_i = \begin{cases} 1, & i = S_F \\ 0, & i \neq S_F \end{cases}, \tag{5}$$

Such hydraulic parameters of a stage as values of its pressure and flows are interconnected by following equations:

$$G'_{Fi} = f\left(P_{Fi}\right) \tag{6}$$

$$G'_{Pi} = f\left(P_{Pi}\right) \tag{7}$$

$$G_{Wi} = f\left(P_{Wi}\right) \tag{8}$$

The frequency rotation of the GC rotors and the temperature of equipment operation mode are assumed constant.

1.3. Basic equations describing the nonstationary processes

Basic equations of nonstationary hydraulic processes are balance equations of process gas in all capacities:

$$\begin{cases} \dfrac{\mathrm{d}H_{Mi}}{\mathrm{d}t} = G'_{Fi} - G'_{Pi} - G'_{Wi} \\ \dfrac{\mathrm{d}H_{Fi}}{\mathrm{d}t} = G_{Fi} - G'_{Fi} \\ \dfrac{\mathrm{d}H_{Wi}}{\mathrm{d}t} = \begin{cases} G'_{Wi} - W - G_{zW}, & i = 1 \cdot \\ G'_{Wi} - G_{Wi}, & i = \overline{2;S} \end{cases} \\ \dfrac{\mathrm{d}H_{Pi}}{\mathrm{d}t} = \begin{cases} G'_{Pi} - G_{Pi}, & i = \overline{1;S-1} \\ G'_{Pi} - P - G_{zP}, & i = S \end{cases} \end{cases} \tag{9}$$

The task of calculation the parameters of nonstationary separation processes is reduced to solution differential equation system (9) of first order with initial conditions (values of pressure in the initial time). The values of flows and holdups are arbitrary functions of the time; the system (9) is nonlinear. These circumstances make impossible the analytical solution of the task set in general case.

2. The solution algorithm of nonstationary separation equations

We consider the capacity with the holdup H. Total flow G_{in} feds to the capacity, the flow G_{out} left out from the capacity.

Differential equation from the system (9) describing non-stationary hydraulic processes in this capacity is written in the general form as:

$$\frac{\mathrm{d}H}{\mathrm{d}t} = G_{\text{in}} - G_{\text{out}} . \tag{10}$$

The value of capacity holdup has been calculated by following equations:

$$H = a \cdot P , \tag{11}$$

$$a = \frac{\mu V}{RT} , \tag{12}$$

where a is specific capacity holdup, kg·Pa^{-1}; P is pressure of process gas into the capacity, Pa; $R = 8{,}314$ J·mole^{-1}·K^{-1} is universal gas constant.

Differentiating the equation (12) we have had:

$$\frac{\mathrm{d}H}{\mathrm{d}t} = a\frac{\mathrm{d}P}{\mathrm{d}t} . \tag{13}$$

The changes of capacity holdup are directly proportional to changes of pressure. It depends on values of flows Gin and Gout which are proportional to the pressure P:

$$a\frac{\mathrm{d}P}{\mathrm{d}t} = G_{\text{in}} - G_{\text{out}} . \quad (14)$$

Replacing derivatives to difference equations by backward Euler method [8] and obtaining the equations (10), (11), (14) on the k-th time layer (at the point in time $t^{(k)}$), we have received:

$$a\frac{P^{(k)} - P^{(k-1)}}{\Delta t} = G_{\text{in}}\left(P^{(k)}\right) - G_{\text{out}}\left(P^{(k-1)}\right), \quad (15)$$

$$\Delta t = t^{(k)} - t^{(k-1)}, \quad (16)$$

where Δt is time step; k is the index of time layer.

Knowing pressure on previous (k-1)-th time layer (at the point in time $t^{(k-1)}$), we have solved derived nonlinear algebraic equation and have found values of pressure in the point of time $t^{(k)}$. The calculation have been realized as iterative process: on each iteration cycle calculation of pressure and flows have been done from first stage to S-th stage. The initial approximation on k-th time layer is the values of pressure and flows on previous (k-1)-th time layer.

Thus the calculation of nonstationary hydraulic processes reduces to replacement differential equations of first order by difference equations, solution of derived nonlinear algebraic equations and iterative evaluation of pressures in each capacity and flows on every time layers satisfying balance equation of process gas into cascade:

$$\left|\frac{\left(F^{(k)} - P^{(k)} - W^{(k)}\right)\cdot \Delta t}{H'^{(k)} - H'^{(k-1)}} - 1\right| \le \sigma , \quad (17)$$

$$H'^{(k)} = \sum_{i=1}^{S}\left[H_{Mi}^{(k)} + H_{Fi}^{(k)} + H_{Wi}^{(k)} + H_{Pi}^{(k)}\right], \quad (18)$$

where H' is the cascade holdup, kg; σ – the condition of iteration process end.

We have realized the algorithm described herein as software product, developed on Delphi programming language using Embarcadero Delphi XE2.

The developed mathematical model has been tested for modeling of nonstationary hydraulic processes in cascades for separation of Si, Xe, Ni and W isotopes. The deflections between estimated and real values are 7.5 %. As the result we have ascertained that developed model is universal for the calculation of nonstationary hydraulic processes in gas centrifuge cascade for separation of multicomponent isotope mixtures using different process gases.

3. Conclusion

1. The result of research is creation of mathematical model of nonstationary hydraulic processes in gas centrifuge cascade for separation of multicomponent isotope mixtures, representing the differential equation system of first order with initial conditions.
2. The solution algorithm of equation system described nonstationary separation processes is developed and realized as software product.
3. We have made the calculation parameters of nonstationary hydraulic processes in GC cascade for separation of Si, Xe, Ni and W isotopes.
4. We have ascertained that developed model is suitable for the calculation of nonstationary hydraulic processes in gas centrifuge cascade for separation of multicomponent isotope mixtures using different process gases.

IOP Conf. Series: Materials Science and Engineering **142** (2016) 012033 doi:10.1088/1757-899X/142/1/012033

References

[1] Cohen K 1951 *The Theory of Isotope Separation as Applied to the Large-Scale Production of U-235* (New York: McGraw Hill)
[2] Sulaberidze G A *et al* 2011 *Theory of cascades for separation of binary and multicomponent isotope mixtures* (Moscow: MEPhI) p. 368
[3] Vlasov V A, Butov V G, Goldobin D N, Orlov A A, Timchenko S N Modeling of nonstationary processes in gas centrifuge cascades 2007 *Tomsk Polytechnic University news* **310** 103
[4] Vlasov V A, Orlov A A, Butov V G, Timchenko S N Modeling of nonstationary hydraulic processes in gas centrifuge cascades for uranium isotopes separation 2009 *Tomsk Polytechnic University news* **315** 94
[5] Orlov A A, Timchenko S N, Sidorenko V S Mathematical Model of Non-Stationary Hydraulic Process Occurring in Gas Centrifuges for Uranium Enrichment 2015 *Advanced Materials Research* **1084** 673
[6] Filimonov S V, Skorynin G M, Goldobin D N Modeling of nonstationary processes in automatic control system of industrial gas centrifuge cascade for uranium enrichment 2004 *Universities news. Physics* **47** 173
[7] Filimonov S V, Skorynin G M, Orlov A A, Goldobin D N Modeling of nonstationary hydraulic processes in industrial gas centrifuge cascade for uranium enrichment 2006 *Tomsk Polytechnic University news* **309** 85
[8] Pirumov U G 2003 *Numerical methods* (Moscow: Drofa)