### GLASS MELT HOMOGENIZATION IN A GLASS FURNACE – MATHEMATICAL AND PHYSICAL MODEL

STANISLAV KASA, ANTONÍN LISÝ

Institute of Glass and Ceramics, Institute of Chemical Technology, Technická 5, 166 28 Prague 6

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The glass melt homogenization process in the furnace melting zone is very important from the standpoint of final glass quality. The paper deals with the effect of locating and connecting of heating electrodes on homogenization in an all-electric tank furnace, using the methods of mathematical and physical modelling. The outputs obtained from both types of models allowed the so-called response curves to be plotted. The curves yield characteristics providing information on the homogenization process. The first part of the paper is concerned with deriving a two-dimensional mathematical model in the form of a partial differential equation and with the procedure for its numerical solving. The second part describes treatment of the homogenization process by physical modelling. The results showed a very satisfactory agreement of the two types of modelling. The effect and configuration and wiring of electrodes on the homogenization process in an all-electric glass tank furnace is evaluated in the conclusion.

### 1. INTRODUCTION

Glass manufacture has been known for several thousand years, but till recently depended solely on empirical knowledge. It was the development of machine production which brought about research of processes taking place in the course of the entire glassmaking procedure, starting with batch preparation and ending with final treatment and finishing of the products. Like in other industries, quality of products plays an important part, and together with energy consumption is the subject of primary interest of all glass manufactures.

However, there has not yet been, and is not likely to be found in the nearest future, any standard criterion for assessing the quality of the glass melt being produced, which would express its quality by a single objective characteristic [1]. And so the quality is described by the following three factors:

- a) degree of melting;
- b) degree of refining;

c) glass homogeneity: in this case, no objective measure is known so that it has to be assessed by a well measurable property such as the refractive index.

The final quality of glass is obviously determined for the most part by the processes taking place in the glass furnace. The quality and thus also the homogeneity of glass is known to be strongly affected by the flow of glass in the furnace and by the parameters affecting the flow, such as the furnace design, the thermal barrier, and in the case of electric heating, also the shape, arrangement and wiring of electrodes in the furnace tank.

The pulse-and-response method, sometimes also called the response curve method, is one of those frequently used in the seeking of suitable designs of glass tank furnaces and in the study of glass flow [2]. The theory of the method was worked out for chemical reactors by Danckwerts [3] and Levenspiel [4]. As the tank furnace is in principle also a kind of continuous reactor, the theory was utilized by Cooper for explaining the processes taking place in a glass tank furnace [5]. A number of other authors also used the pulse-and-response method to describe the behaviour of glass furnaces [6–16]. All of these studies were concerned with the use of this method directly on the furnaces. Very valuable results were presented by Smrček [12–16] who was the only author to apply the method to comparing and evaluating the performance characteristics of various types of glass furnaces.

The literature quoted above indicates that the implementation of the pulse-and-response method for the purpose of determining the performance characteristics of glass furnaces is a quite demanding task. For this reason, some authors [17–22] supplement the respective solutions with those obtained from mathematical models of the melting process, and with homogenization models, including calculation of the time dependence of concentration distribution of a tracing substance at a given point. This represents calculation of response curves which can be obtained on the actual furnace by the pulse-andresponse method. The mathematical modelling of homogenization has the primary advantage of a great variety of solutions, available by mere setting of various initial and boundary conditions. Such a variability is of course unviable with actual furnaces, also because it would frequently result in emergency operational situations.

The present study had the objective to construct a two-dimensional mathematical model of the homogenization process in an all-electric glass furnace and to assess the effect of the configuration of electrodes on homogenization. The model was worked out so as to allow response curves to be plotted from the results, and to evaluate the homogeneity in the melting zone



Fig. 1. Volume element  $\Delta x \Delta y \Delta z$ , stationary in space through which component A is passing. 1 – wall at x; 2 – wall at  $x + \Delta x$ .

according to the curve parameters. As the respective mathematical models require the speed vector components at the individual points of the space investigated to be known, a physical model was also run to provide the speed vector of the components, determined from videorecordings of the flow. The physical model was also used to investigate the effect of the electrode configuration on the homogenization process in the melting zone of the furnace, and this allowed the results yielded by the two models to be compared.

### 2. TWO-DIMENSIONAL MATHEMATICAL MODEL

To derive a two-dimensional mathematical model of the homogenization process, i.e. a partial differential equation describing convective diffusion, use was made of the mass conservation law for component A (indicator) per volume element  $\Delta x \Delta y \Delta z$ , immobile in space passed through by a binary mixture of components A and B (glass melt, model liquid). On the assumption that components A and B do not react and that component A is not produced by a chemical reaction, one may write the following expressions for the individual contributions to the mass balance in a volume element, according to Fig. 1:

- the rate of change in the mass of component A in a volume element:

$$\frac{\partial \rho_{\mathbf{A}}}{\partial \tau} \Delta x \Delta y \Delta z$$

- supply of component A through the wall at x:

 $n_{\rm A}x/x\Delta y\Delta z$ 

- discharge of component A through the wall at  $x + \Delta x$ :

### $n_{\rm A}x/x\Delta x\Delta y\Delta z$ .

Similarly, it is possible to write expressions for the entry and exit of component A through the other walls of the volume element, i.e. in directions y and z. On substituting the flux density  $A(n_A)$  by a term containing concentration gradients, i.e. the formulation of the first Fick law for binary diffusion [23], one obtains the diffusion equation which can be writen in the form

$$\frac{\partial c_{\mathbf{A}}}{\partial \tau} + (\nabla c_{\mathbf{A}} w) = \nabla c D_{\mathbf{A}\mathbf{B}} \nabla x_{\mathbf{A}}$$
(1)

where  $x_A$  is a molar fraction for which it holds that

$$x_{\rm A} = \frac{c_{\rm A}}{c} \,. \tag{2}$$

Using justified simplifications such as a constant density, a constant total molar concentration of a constant diffusion coefficient [24], equation (1) can be adjusted to the following form:

$$\frac{\partial c_{\mathbf{A}}}{\partial \tau} + (\boldsymbol{w} \nabla c_{\mathbf{A}}) - D_{\mathbf{A}\mathbf{B}} \nabla^2 c_{\mathbf{A}} = 0.$$
(3)

Equation (3) finds successful use in the solving of diffusion processes in dilute solutions, and can therefore be also employed in describing the homogenization process in glass tank furnaces [18, 20, 21, 22], and in its treatment by means of both mathematical and physical models.

### 3. NUMERICAL SOLUTION OF EQUATION (3)

In the present case, equation (3) was solved in two spatial dimensions (x and y) and the time dimension  $(\tau)$ . For this purpose, it was written in the form

$$\frac{\partial c}{\partial \tau} + w_x \frac{\partial c}{\partial x} w_y \frac{\partial c}{\partial y} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right). \tag{4}$$

The aim was to find a function of  $c(x, y, \tau)$  conforming to differential equation (4) for initial conditions (5) and boundary conditions (6). The initial conditions  $(\tau = 0)$ :

$$c = 1 \text{ for } y = 0; \ 0 \le x \le x_k \tag{5}$$

$$c = 0 \text{ for } 0 < y \leq y_k; \ 0 \leq x \leq x_k.$$

The boundary conditions:

$$c = 0 \text{ for } \tau > 0; \ y = 0; \ 0 \le x \le x_k$$

$$\frac{\partial c}{\partial x} = 0 \text{ for } \tau > 0; \ 0 \le y \le y_k; \ x = 0; \ x = x_k$$

$$\frac{\partial c}{\partial y} = 0 \text{ for } \tau > 0; \ y = y_k; \ 0 \le x \le x_k .$$
(6)

The two-dimensional mathematical model was processed by a computer, using the Fortran language. The computer program was composed into ten interconnected blocks:

block 1: planting of input quantities;

- block 2: calculation of constants A, B, C, E,  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\delta$ , in the individual nodal points of the grid at time  $\tau = 0$ ;
- block 3: subroutine ensuring the occupancy of matrix A and matrix B for the initial conditions;
- block 4: subroutine for solving a system of linear equations by Gauss'es elimination method using main element selection;
- block 5: calculation of constants (cf. block 2) in the individual nodal points of the grid at time  $\tau > 0$ ;

block 6: subroutine ensuring occupancy of matrix A and matrix B at time  $\tau > 0$ ;

block 7: cf. block 4;

- block 8: calculation of the solution standard;
- block 9: alternative box deciding on attainment of desired accuracy;

block 10: entry of results into the output file. Input quantities of the computer program:

- size of grid covering the chosen section of the furnace model;
- diffusion coefficient of the indicator in the model liquid;
- time step;
- solution accuracy required;
- components (x and y) of convective flow rate vectors at the individual nodal grid points, obtained by measuring the flow rate fields on the physical model.

Output quantities of the computer program:

 matrix of indicator concentrations at the nodal points of the grid serving in the determination of response curves.

### 4. PHYSICAL MODEL

To model the homogenization process by means of a two-dimensional mathematical model one has to know the components of the flow rate vectors at the individual nodal points of the grid covering the region being investigated in the melting zone. For this purpose, use was made of a physical model allowing the flow in the melting zone to be followed and the respective components of the flow rate vectors established. The physical model was also used to monitor the course of homogenization in the melting zone in terms of the electrode configuration, using the response curve method. The results obtained from the two models could thus be compared. As the task was to study the effect of electrode configuration on the homogenization process, a physical liquid model of an all-electric furnace on a 1 : 16 scale was constructed so as to permit various configurations of rod and plate electrodes to be arranged, in both horizontal and vertical positions. A schematic diagram of the physical model is shown in Fig. 2. Fig. 3 depicts the configurations of electrodes for the individual variants studied on the physical model and also dealt with by the mathematical model. The design of the physical model also made it possible, for the purposes of the response curve method, to place on the liquid surface a continuous strip of strongly coloured model liquid (indicator) and to take samples of the model liquid



Fig. 2. Schematic diagram of the physical model of the melting furnace. 1 - the place where the indicator is introduced; 2 - the place where the model liquid samples are taken.



Fig. 3. Schematic diagram of the arrangement and wiring of electrodes for the individual variants. 1 - variant 1; 2 variant 2; 3 - variant 3 and 4.

at the exit from the melting zone at regular intervals, as illustrated by Fig. 3.

### 5. INDICATORS

The flow and mixing of the model liquid in the physical model is best simulated by means of coloured indicators. A complete range is known, but only some nem are suitable. Selection of suitable coloured ind ators for the purposes of modelling the response curves, including determination of their diffusion cofficients in model liquids, was described in detail in [24, 26, 27]. For the glycerine-borax model liquids, the best results were obtained with two indicators, namely

a) Neutral Red –  $C_{15}H_{17}N_4Cl$ 

$$CH_{3} \bigvee_{\substack{N \\ CH_{3}}} -N = \bigvee_{\substack{N \\ CH_{3}}} -N = \bigvee_{\substack{N \\ CH_{3}}} -NH_{2}$$

b) Malachite Green - C<sub>23</sub>H<sub>25</sub>N<sub>2</sub>Cl

whose diffusion coefficients change little with temperature, so that they may be considered to be constant over the temperature interval of the physical model. The following values of diffusion coefficients were taken over from [27] for the mean temperature of 50°C:

- Neutral Red  $D = 5 \times 10^{-8} \text{ cm}^2 \text{s}^{-1}$  Malachite Green  $D = 1 \times 10^{-7} \text{ cm}^2 \text{s}^{-1}$ .

Malachite Green was finally chosen, because it exhibited a better dependence of absorbance on the wavelength of the light employed. This aspect was important since the samples of the dyed model liquid were immediately tested on a spectrophotometer after being taken at the outlet from the melting zone. This allowed the time dependence of changes in the relative concentrations of the indicator to be determined. A stock solution having a relative concentration  $c_{rel} = 1$  was prepared by mixing the indicator with the model liquid, and placed onto the surface in the model.

### 6. THE SIMILARITY OF CONVECTIVE FLOW

The homogenization process in the melting zone was described by means of equation (3), derived for convective diffusion. For this reason the conditions in the model had to be adjusted in a way ensuring similarity of convective flow in the model to that in the furnace. According to [28], such a similarity is ensured by equality of Grashof's number. As an equality of Galilei's number was likewise attained, a sufficient condition for validity is provided by the equation.

$$[\beta \Delta T]_{M} = [\beta \Delta T]_{D} \quad . \tag{7}$$

In this case, the following values were substituted into (7):

$$\beta_M = 4.94 \times 10^{-4} \text{ K}^{-1}$$
  $\beta_D = 6.62 \times 10^{-5} \text{ K}^{-1}$   
 $\Delta T_M = 27.1 \text{ K}$   $\Delta T_D = 200 \text{ K}$ 

then

 $[\beta \Delta T] = 0.0134$ 

and

 $[\beta \Delta T] = 0.0132$ 

so that the convective flow in the model simulates very well that in the furnace.

### 7. THE VALUES MEASURED

As stated already in Chapter 4, the physical model had the following purposes: a) To determine the flow rate vector components at the nodal points (entry into the two-dimensional mathematical model). b) To determine the response curves for the configurations and ways of wiring of electrodes being studied.

As far as point a) is concerned, the region investigated, i.e. a vertical section through the longitudinal tank axis (cf. Fig. 2) was covered by a square grid with  $9 \times 20$  nodal points.

As regards point b), four variants whose arrangement is shown in Table I, were measured on the physical model.

Table II lists the values of flow rates and flow directions at the individual nodal points of the grid, established by measurement on the physical model for variant 1. Only one half of the values are given because of the symmetry involved. The upper data is the rate of flow in the model in cm s<sup>-1</sup>, the lower one being the direction of flow in degrees, oriented according to Fig. 4. The data for variants 2 through 4 is available at the authors' place of business.

Arrangement of the experimental variants on the physical model

Variant	Electrode type	Electrode input [W]
1	rods, vertical	92.2
2	plates	89.1
3	plates	71.6
	rods, horizontal	38.3
4	plates	57.5
	rods, horizontal	57.7



Fig. 4. Orientation of the flow rate vectors at the nodal points of the grid.

Tables III and IV list the time dependence of relative indicator concentrations at the outlet from the melting zone, established for variant 1 on the physical model and calculated from the mathematical model. The data for variants 2, 3 and 4 is also kept at the authors'.

The time dependences of the relative indicator concentrations at the outlet from the melting zone are plotted for all the variants in Fig. 5 (for the physical model) and in Fig. 6 (for the mathematical model).

### 8. EVALUATION OF THE RESPONSE CURVES AND THE RESULTS

The given time dependence of the relative concentrations of the indicators were evaluated for the individual variants on the basis of the following characteristics:

a) Delay, characterizing the mean time of residence of the liquid in the system, for which it holds that

$$\tau_{\rm s} = \frac{\sum c_i \tau_i}{\sum c_i} \tag{8}$$

b) Dispersion, characterizing the degree of homogeneity of the liquid in the system, for which it holds that

$$\sigma = \frac{\sum \Theta_i^2 E_i}{\sum E_i} - 1, \qquad (9)$$

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j i	2	3	4	5	6	7	8	9	10
2	0.038	0.096	0.970	0.061	0.042	0.038	0.031	0.048	0.057
	210	120	60	30	0	0	330	310	290
3	0.030	0.109	0.112	0.086	0.079	0.042	0.038	0.052	0.063
	270	90	90	70	50	10	340	300	270
4	0.025	0.128	0.130	0.072	0.025	0.001	0.016	0.054	0.068
	270	90	90	80	85	0	265	270	270
5	0.025	0.115	0.118	0.081	0.054	0.043	0.041	0.051	0.061
	270	90	90	100	110	170	180	210	260
6	0.023	0.109	0.111	0.072	0.038	0.031	0.025	0.047	0.058
	270	90	90	110	140	170	180	220	240
7	0.020	0.095	0.098	0.048	0.031	0.025	0.019	0.031	0.042
	300	90	90	130	150	165	170	180	190
8	0.018	0.067	0.072	0.034	0.025	0.012	0.009	0.011	0.013
	0	80	100	150	160	170	175	180	180

### Table II

The rates of flow cm  $s^{-1}$  and their directions at the grid nodal points (Variant 1)

## Table III

Time dependence of relative indicator concentrations at the outlet of the melting zone - physical model (Variant 1)

au [h]	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
$c_{rel}$	0.43	0.76	0.82	0.83	0.77	0.65	0.50	0.41	0.35
τ [h]	5.5	6.0	6.5	7.0	7.5	8.0	8.5	9.0	9.5
c <sub>rel</sub>	0.30	0.27	0.24	0.22	0.20	0.18	0.17	0.16	0.14
τ [h]	10.0	10.5	11.0	11.5	12.0	12.5	13.0	13.5	14.0
<sub>Crel</sub>	0.13	0.11	0.10	0.09	0.08	0.07	0.06	0.05	0.05
τ [h] c <sub>rel</sub>	14.5 0.05	15.0 0.05							

### Table IV

Time dependence of relative indicator concentrations at the outlet of the melting zone – mathematical model (Variant 1)

τ [h]	1.00	1.25	1.43	1.70	1.95
<sub>Crel</sub>	$0.35 \times 10^{-3}$	$0.70 \times 10^{-3}$	$0.119 \times 10^{-2}$	$0.171 \times 10^{-2}$	$0.215 \times 10^{-2}$
τ [h]	2.20	2.50	2.83	3.18	3.55
<sub>Crel</sub>	$0.25 \times 10^{-2}$	$0.27 \times 10^{-2}$	$0.276 \times 10^{-2}$	$0.271 \times 10^{-2}$	$0.262 \times 10^{-2}$
τ [h]	4.00	4.45	5.10	5.85	6.75
<sub>Crel</sub>	$0.25 \times 10^{-2}$	$0.238 \times 10^{-2}$	$0.22 \times 10^{-2}$	$0.203 \times 10^{-2}$	$0.184 \times 10^{-2}$
τ [h] <sub>Crel</sub>	$7.85 \\ 0.16 \times 10^{-2}$	8.98 $0.14 \times 10^{-2}$	$ \begin{array}{c} 10.1 \\ 0.122 \times 10^{-2} \end{array} $	$     11.25 \\     0.107 \times 10^{-2} $	12.5 0.927 × 10 <sup>-3</sup>



Fig. 5. Time dependence of the relative concentrations of the indicator at the outlet from the melting zone. Physical model: 1 - variant 1; 2 - variant 2; 3 - variant 3; 4 - variant 4.

where

$$E_{i} = \tau_{s} \frac{\sum c_{i}}{\sum (c_{i} \Delta \tau_{i})}$$
(10)

$$\Theta_i = \frac{\tau_i}{\tau_s} \tag{11}$$

$$\Delta \tau_i = \tau_{i+1} - \tau_i \,. \tag{12}$$

In both (8) and (12), the substripts i are related to the time step.

Enumeration of equations (8) through (12) by means of data obtained from the physical and the mathematical model yielded the results listed in Table V.

### 9. CONCLUSION

The following conclusions can be formulated on the basis of results yielded by the two types of models:

- 1) Both the physical and the mathematical model allow the effect of electrode configuration and wiring on the homogenization effect in the furnace melting zone to be followed.
- 2) The two models show a satisfactory agreement of results, so that the conclusions given below hold for both types of models.
- 3) The variants with vertical electrodes in the tank bottom, compared to those with plate-shaped electrodes or a combination of plate-shaped and



Fig. 6. Time dependence of the relative concentration of the indicator at the outlet from the melting zone. Mathematical model: 1 - variant 1; 2 - variant2; 3 - variant 3; 4 - variant 4.

horizontal rod electrodes, yield lower values, which means that rod electrodes cut down the residence time in the furnace melting zone.

4) Dispersion values are higher with variants using vertical rod electrodes. This indicates that the presence of vertical electrodes in the melting zone contributes more efficiently to intensifying the mass transfer and thus also the homogeniz-

### Table V

The results yielded by the physical model and the mathematical model

Model	Variant	τ. [h]	σ	$ au_{ extsf{max}} [ extsf{h}]$	τ <sub>0</sub> [h]
physical	1 2 3 4	4.21 4.79 5.03 5.58	0.87 0.83 0.69 0.53	2.7 2.5 3.3 4.8	0.6 0.9 0.9 1.2
mathe- matical	1 2 3 4	3.97 4.25 4.59 5.15	0.81 0.79 0.62 0.46	2.4 2.8 2.9 4.5	0.7 0.8 0.9 0.9

ing process than do the plate-shaped or horizontal rod electrodes.

5) The value of  $\tau_s$  i.e. the time at which the first traces of the indicator are recorded at the outlet, are lowest with variant 1, i.e. that with vertical electrodes. This is indicative of the presence of extensive flow in the melting zone, and thus of very good conditions for homogenization.

I hay therefore be summarized that the use of Ver al rod electrodes in the heating zones of allelectric glass tank furnaces provides more favourable conditions for the homogenization process than the application of plate-shaped electrodes or vertical rod electrodes.

### List of symbols

- T Cartesian coordinates [m]
- Cartesian coordinates [m] y
- Cartesian coordinates [m] z
- mass flow density of a component  $[kg m^{-2}s^{-1}]$ n
- time [s]  $\boldsymbol{\tau}$
- rate of flow  $[m s^{-1}]$ w
- $\nabla$
- operator "nabla"  $[m^{-1}]$ diffusion coefficient  $[m^2s^{-1}]$ D
- concentration [mol  $m^{-3}$ ] С
- mass concentration of component  $i \, [\text{kg m}^{-3}]$  $\rho_i$
- density  $[kg m^{-3}]$ ρ
- depth of model tank [m] TL
- length of model tank [m] Yk

- h lengthwise step in directions x and y [m]
- k time step [s]
- $c_k$  concentration at k-th time step [mol m<sup>-3</sup>]
- $c_{k+1}$  concentration at k+1 th time step [mol m<sup>-3</sup>]

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### HOMOGENIZACE SKLOVINY VE SKLÁŘSKÉ TAVICÍ PECI – MATEMATICKÝ A FYZIKÁLNÍ MODEL

### STANISLAV KASA, ANTONÍN LISÝ

### Ústav skla a keramiky, Vysoká škola chemicko-technologická, Technická 5, 166 28 Praha 6

Kvalita vyráběné skloviny patří mezi nejvíce sledované parametry u všech výrobců skla. Neexistuje však jednotné kritérium pro hodnocení kvality vyráběné skloviny a proto se zatím vyjadřuje pomocí tří ukazatelů. Jsou to stupeň utavení, stupeň vyčeření a homogenita skloviny. Z toho plyne, že výsledná kvalita skla je dána procesy, které probíhají v tavicí peci a proto také kvalitu skloviny ovlivňuje řada parametrů mající vliv na tyto procesy, tj. konstrukční řešení pece, umístění a mohutnost tepelné bariéry a u celoelektrických pecí také rozmístění a zapojení elektrod v tavicím bazénu pece. Jednou z metod pro vyšetřování vlivu výše uvedených parametrů na proces homogenizace je metoda odezvových křivek, jež byla zpočátku vypracována pro chemické reaktory. Jelikož sklářská tavicí pec je také reaktor, je možné zmíněnou teorii i zde využít. V poslední době se k vyšetřování procesu homogenizace také užívá metoda modelování umožňující provádět výpočty a sledování časových závislostí rozdělení koncentrací stopovací látky v tavicí části pece nebo modelu.

V našem případě byl sestaven jak dvourozměrný matematický model, tak i model fyzikální umožňující sledovat proces homogenizace. Bylo také provedeno jejich vzájemné porovnání. V první části příspěvku je pojednáno o matematickém modelu procesu homogenizace. Je ukázán postup odvození matematického modelu a jeho následné numerické dvourozměrné zpracování za použití počátečních a okrajových podmínek.

Ve druhé části je popsáno použití fyzikálního kapalinového modelu celoelektrické tavicí pece při určení složek vektorů rychlostí v uzlových bodech sítě (vstup do modelu matematického) a při vyšetřování vlivu konfigurace a zapojení elektrod na proces homogenizace pomocí metody odezvových křivek. Vyhodnocení odezvových křivek získaných z matematického a fyzikálního modelu pro jednotlivé konfigurace elektrod je uvedeno v tabulce 5. Z údajů v této tabulce vyplývá jednak velmi dobrá shoda mezi výsledky matematického a fyzikálního modelu a jednak skutečnost, že svislé elektrody ze dna tavicího bazénu pece příznivěji působí na proces homogenizace než ostatní proměřované konfigurace elektrod, neboť výrazněji přispívají k intenzifikaci přenosu hmoty.

- Obr. 1 Objemový element  $\Delta x.\Delta y.\Delta z$  nehybný v prostoru jímž prochází složka A. 1 – stěna při x; 2 – stěna při  $x + \Delta x$ .
- Obr. 2. Schéma fyzikálního modelu tavicí pece. 1 místo vkládání indikátoru; 2 – místo odběru vzorků modelové kapaliny.
- Obr. 3. Schéma rozmístění a zapojení elektrod pro jednotlivé varianty. 1 – Varianta 1; – 2 – Varianta 2; 3 – Varianta 3 a 4.
- Obr. 4. Orientace vektorů rychlostí v uzlových bodech sítě.

- Obr. 5. Časové závislosti relativních koncentrací indikátoru na výstupu z tavicího prostoru – fyzikální model:
  1 – Varianta 1; 2 – Varianta 2; 3 – Varianta 3; 4 – Varianta 4.
- Obr. 6. Čarové závislosti relativních koncentrací indikátoru na výstupu z tavicího prostoru – matematický model: 1 – Varianta 1; 2 – Varianta 2; 3 – Varianta 3; 4 – Varianta 4.

# **Recenze knih**

QUANTITATIVE MINERAL ANALYSIS OF CLAYS. Eds.: D. R. Pevear, F. A. Mumpton. The Clay Minerals Society, Evergreen (Colorado) 1989. 171 stran, 54 obr.

Jako první svazek řady Seminárních přednášek americké Společnosti jílových minerálů byla tato knížka sestavena z přednášek, jež odezněly na Semináři o kvantitativní modální analýze jílů, konaném r. 1985 v Denveru ve státě Colorado.

Dílo sestává ze šesti kapitol:

- Teorie a praxe rentgenové difrakční kvantitativní fázové analýzy jílových minerálů 34 str. (R. C. Reynolds);
- Počítačový program pro semikvantitativní rtg difrakční analýzu minerálního složení – 14 str. (J. W. Hosterman a F. T. Dulong);
- Vyrovnávání a rozklad rtg difrakčních profilů pomocí samočinného počítače – 51 str. (R. C. Jones);
- Kvantitativní modální analýza na základě měřené absorpce rtg záření a rtg difrakce 15 str. (B. L. Davis a L. R. Johnson);
- Kvantitativní určování jílů a jiných nerostů v horninách - 33 str. (M. Slaughter);
- Kombinace rtg difrakce a analýzy prvkového složení pro kvantitativní stanovení minerálů v geologických vzorcích - 12 str. (C. S. Calvert, D. A. Palkowsky a D. R. Pevear)
- a dodatku
  - Šablony pro konverzi 2θ na mezirovinné vzdálenosti, zhotovované samočinným počítačem – 4 str. (L. C. Poppe a J. E. Dodd).

První kapitola podává celkový popis metody kvantitativní rtg difrakční fázové analýzy orientovaných jílových agregátů. Jsou diskutovány teoretické i praktické aspekty této techniky a kriticky se hodnotí její možnosti. Podrobně se pojednává o přednostní orientaci a o intensitních faktorech. V druhé kapitole je popisován počítačový program vyvinutý Geologickým průzkumem USA pro vyhlazení digitálních údajů, odstranění pozadí, vyhledávání a identifikaci píků a určování koncentrací až 12 minerálů v analyzovaném vzorku. Jiný program, vytvořený na Havajské univerzitě v Honolulu a nesoucí exotický název Pi' o Pili Pa'a (což prý znamená "prokládání křivky" v nářečí havajských domorodců) je uváděn ve třetí kapitole. Je zde zasazen do kontextu vynikajícího přehledného referátu o prokládání křivek, dekonvoluci a rozkladech. Tato kapitola je nejrozsáhlejší a pravděpodobně také nejcenější součástí textu. Čtvrtá kapitola popisuje tzv. metodu referenčních intenzit vyvinutou Briantem L. Davisem, jež kombinuje rtg difrakci s měřením absorpce rentgenového záření. Specifické pro tento postup je, že využívá uspořádání na průchod a zvláštním, důmyslným preparačním postupem eliminuje vliv přednostní orientace. Zdá se, že tato metoda - byť poněkud pracná - je nejpřesnější a nejspolehlivější technikou kvantitativní rtg difrakční analýzy fázového složení práškových vzorků. Určovat kvantitativně zastoupení jílových minerálů je obtížné, protože tyto minerály obsahují rozličné strukturní defekty a mají proměnlivé prvkové složení. Využitím informace o chemismu můžeme proto účinnost kvantitativní rtg difrakční analýzy fázového složení jílů podstatně zvýšit. To se vysvětluje v posledních dvou kapitolách, jež uvádějí na řadě příkladů jak účinně kombinovat rtg difrakci s chemickou analýzou prvkového složení, určením specifického povrchu a schopnosti výměny kationtů.

Kniha je velmi zdařilá a moderností svého pojetí, šíří záběru, jakož i podrobností zpracování problematiky rtg difrakční kvantitativní analýzy fázového složení jedinečná. Ačkoli pojednává o jílech – a vlastně asi právě proto, že pojednává o jílech, jejichž fázová analýza je snad vůbec nejtvrdším oříškem – bude tato kniha užitečná pro každého, kdo se zabývá kvantitativní fázovou analýzou – nebo alespoň využívá výsledky takových rozborů – bez ohledu na to, jaké látky zkoumá.

Knihu lze objednat na adrese sekretariátu společnosti: The Clay Minerals Society, P.O.Box 4416, Boulder, Colorado 80306, USA.

> Jaroslav Fiala Ústřední výzkumný ústav ŠKODA, 316 00 Plzeň