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Thermal behavior of absorbing and scattering glass media containing molecular water impurity

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Abstract

The effect of the presence of molecular water impurity of various concentrations in absorbing and scattering glass media on the temperature field in a layer subjected to thermal infrared radiation is investigated. The analysed medium is treated as a multicomponent medium consisting of glass matrix and water impurity. The effect of radiation on the medium is expressed by heat sources in each component due to absorption of radiation. It is shown that the presence of water impurity in the glass medium should be accounted for in order to predict the temperature distribution during radiation action. The effect of scattering of radiation by water molecules on thermal and diffusive processes in the analysed medium is shown to be insignificant.

Keywords: Glass; Water impurity; Infrared radiation; Heat and mass transfer; Absorption; Scattering

1. Introduction

In most radiative transfer problems glass materials are treated as one-component media. Absorption coefficient of such media is measured experimentally and usually approximated by a piece-wise homogeneous function. In majority cases such an approximation works well enough for practical applications. In the meantime, most glasses contain impurities in the form of gaseous species whose presence in many cases affects overall behavior of a glass product and often is undesirable as having detrimental effects on many properties of glasses. In particular, it is well known that water impurity increases the optical transmission losses, impairs the characteristics of optical fibers amplifiers [1]. Moreover, water causes deterioration of thermal, chemical and mechanical properties of glasses in general [2].

The presence of gaseous impurity in a semitransparent glass medium becomes even more prominent in the case of incident radiation. This is due to the fact that gaseous impurity usually creates no chemical bonds with glass matrix thus retaining its identity and therefore has its own response to incident radiation which may differ significantly from that of glass matrix. The spectral absorption coefficient of a gaseous impurity in a glass is often higher than that of glass matrix. Together with the fact that, for example, water impurity concentration may reach 0.5–2.3 wt.% in geological glasses [2] and even 1.5–10 wt.% in some aluminosilicate glasses [3], its contribution to thermal state in glass should not be neglected.

Presence of gaseous impurity in glasses implies its mobility within glass matrix. Redistribution of gaseous impurity in a glass due to diffusion may contribute to overall thermal state in glass subjected to radiation. In addition, diffusion of a gaseous impurity in glass due to incident radiation is of independent interest because of aforementioned importance of

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Nomenclature

a	absorption coefficient	m^{-1}
b	asymmetry factor of scattering phase function	
Bi_T	Biot criterium for heat exchange	
Bi_c	Biot criterium for mass exchange	
c	dimensionless admixture concentration	
c_1, c_2	radiative constants	
C	heat capacity	$\mathrm{J \cdot kg^{-1} \cdot K^{-1}}$
D	diffusivity	$\mathrm{m^2 \cdot s^{-1}}$
D_0	diffusion factor	$\mathrm{m^2 \cdot s^{-1}}$
E	molar energy	$\mathrm{J \cdot mol^{-1}}$
E_{act}	diffusion activation energy	$\mathrm{J \cdot mol^{-1}}$
h	thickness of the layer	m
I	radiation intensity	$\mathrm{W \cdot m^{-2} \cdot ster^{-1} \cdot \mu m^{-1}}$
J	intensity of absorption band [12]	$\mathrm{cm^2 \cdot Pa^{-1}}$
J	mass flux	$\mathrm{kg \cdot m^{-2} \cdot s^{-1}}$

Greek symbols

β	direction of radiation propagation in the layer	
$\Delta\omega_{\mathrm{ef}}$	effective width of the absorptive	s^{-1}
θ_{λ_n}	optical thickness of the medium	
κ	thermal diffusivity	$\mathrm{m^2 \cdot s^{-1}}$
λ	wavelength	μm
λ_c	cutoff wavelength	μm
ν	direction cosine of radiation propagation	
ρ	density	$\mathrm{kg \cdot m^{-3}}$
σ	scattering coefficient	m^{-1}
τ_c	dimensionless time in Eq. (12)	
τ_T	dimensionless time in Eq. (11)	
Ω	spectral albedo, $= \frac{\sigma}{a+\sigma}$	
Φ	phase function	
χ	thermal conductivity	$\mathrm{W \cdot m^{-1} \cdot K^{-1}}$

k	coefficient in Eq. (3)	
l	spatial grid for optical length	
M^I	molar weight of impurity	$\mathrm{kg \cdot mol^{-1}}$
M	number of spatial points	
N	number of ordinate directions	
n_λ	refractive index	
P	total number of absorption bands	
Q	power of heat source per unit mass	$\mathrm{W \cdot kg^{-1}}$
$\overline{R}$	universal gas constant	$\mathrm{J \cdot K^{-1} \cdot mol^{-1}}$
R_λ	reflectivity	
t	time	s
T	temperature	K
T_a	ambient temperature	K
w	weight of the quadrature	
z	thickness coordinate	m
$\bar{z}$	dimensionless coordinate, $= z/h$	

Subscripts

j	spatial point
max	maximal value
n	ordinate direction
s	quantity related to surrounding
λ, ω	spectral quantities
0	initial value

Superscripts

atm	value calculated at atmospheric pressure acording to Clapeyron equation
I, M	quantities related to impurity and matrix, respectively

the influence of gaseous impurity on operating efficiency of glass products.

Presence of absorption bands proper for gaseous impurities in absorption spectrum of a glass proves that they retain their identity, at least in terms of radiative properties [3]. Therefore, a more accurate consideration of radiative transfer in glasses requires accounting for their real structure. Consequently, we have to treat such glasses as multicomponent media their components being glass matrix and gaseous impurities.

Importance of diffusion of certain constituents as well as of the difference in the values of absorption coefficients of different constituents is reported in experimental works [4,5] on composites, which represent another type of multicomponent media where individual constituents retain their indentities. In particular, it has been established in [4] that a composite fabricated by microwave radiation sintering has improved mechanical properties over conventionally sintered materials. This has been attributed to an essential difference between values of absorption coefficients of different constituents at high temperature. Similarly, it was shown in [5] that selective absorption by certain constituents promotes solid phase diffusion and actually drops the apparent diffusion activation energy. However, no theoretical models were presented in [4,5] to capture these phenomena. Also, it has been shown in [6] that individual responses to radiation of aluminium particles and solid matrix in a solid composite propellant led to unwanted agglomeration of aluminium particles thus reducing operating efficiency of the product.

Therefore, it is of interest and practical need to develop a model decoupling relative effects of different components in multicomponent media on their overall behavior. This paper contributes to the field by analysing the selective effect of radiation on a multicomponent glass medium. Previous investigations presented in [7,8] are improved here by accounting for radiation scattering by water impurities molecules. A selective effect of radiation is accounted for not only by different thermal states of constituents, but also by a specific water diffusion rate. We investigate the correlation between water impurity concentration and temperature field in fused silica glass subjected to infrared radiation and show that at a certain value of water concentration its presence in glass should be accounted for in order to obtain the accurate prediction of the temperature field.

2. Radiation equations

Presence of an impurity in a semitransparent medium makes the latter optically inhomogeneous resulting in radiation scattering. The radiation transfer equation for a one-dimensional layer in an approximation of a "cold" medium will then appear as [9]

$$\nu\frac{\partial I_\lambda(\bar{z},\nu)}{\partial\theta_\lambda} = -I_\lambda(\bar{z},\nu) + \frac{\Omega_\lambda}{2}\int_{-1}^{1} I_\lambda(\bar{z},\nu_i)\Phi(\nu_i,\nu)\,\mathrm{d}\nu_i$$
$$\nu = \cos\beta \tag{1}$$

At the boundaries $\bar{z}=0$ and $\bar{z}=1$ of the layer we assume conditions of diffuse reflection:

$$I_\lambda(0,\nu) = I_\lambda^{(0)} + 2R_\lambda\int_{-1}^{0}\nu_i I_\lambda(\nu_i)\,\mathrm{d}\nu_i$$
$$I_\lambda(1,\nu) = I_\lambda^{(1)} + 2R_\lambda\int_{0}^{1}\nu_i I_\lambda(\nu_i)\,\mathrm{d}\nu_i \tag{2}$$

In (2) $I_\lambda^{(0)}$, $I_\lambda^{(1)}$ are portions of radiation intensities, leaving respective boundaries of the layer, due to external thermal radiation sources. The sources of thermal radiation from appropriate sides of the layer are heated to certain temperatures$T^{(0)}$, $T^{(1)}$, and their spectral intensities are defined by the well-known Planck's law

$$I_\lambda^{(s)} = k^{(s)}\frac{2n_\lambda^2 c_1}{\lambda^5\exp(c_2/\lambda T^{(s)}-1)},\quad s=0,1,\ k^{(s)}=\text{const} \tag{3}$$

where c_1, c_2 are radiation constants [10] and $k^{(0)}$, $k^{(1)}$ [8] are dimensionless coefficients accounting for the emissivity of the real radiation source as well as for its geometrical position with respect to an irradiated object. In particular case of the radiation source in a shape of infinite surface parallel to an infinite irradiated layer, the coefficient $k^{(s)}$ is simply the emissivity of the radiation source. Coefficients $k^{(0)}$, $k^{(1)}$ are assumed to be independent of the direction of radiation propagation, coordinate and wavelength λ, therefore radiation is homogeneous and diffusive [10].

To get the quantitative solution of the radiation transfer equation one needs to know, among other things, the values of spectral absorption coefficient and phase function. The absorption coefficient for the medium considered here may be taken as a sum of those for glass matrix and water impurity [11]

$$a_\lambda = a_\lambda^M + a_\lambda^I \tag{4}$$

Usually the absorption coefficient of a glass matrix can be approximated within several bands model [12], which divides the entire spectrum range by two or more wide intervals where absorption coefficient has constant values. In the meantime, molecular water is known to absorb radiation in narrow spectral intervals called bands and its absorption coefficient can be written as follows

$$a_\lambda = a_\omega = \frac{J_\omega}{\Delta\omega_{\mathrm{ef}}}$$

where quantity J_ω, calculated per unit frequency interval, and $\Delta\omega_{\mathrm{ef}}$ are intensity and effective width of absorption band [13], respectively. Unlike solids with constant densities, water in glass is represented by separate molecules and thus may have various densities. Since radiation absorption by water in glass is ultimately determined by a number of absorptive centers, i.e., the number of molecules, the water absorption coefficient should necessarily depend upon its density in glass. This dependence may be accepted linear [11]. Then treating water vapor density ρ^w at atmospheric pressure (ρ^w_{atm}) as the reference density, we obtain

$$a_\lambda = \frac{J_\omega^{\mathrm{atm}}}{\Delta\omega_{\mathrm{ef}}^{\mathrm{atm}}}\frac{\rho^w}{\rho^w_{\mathrm{atm}}}$$

Introducing dimensionless water mass concentration $c=\rho^I/\rho$ (where ρ^I and ρ are density of water impurity and total density of glass medium, respectively) in the last expression yields

$$a_\lambda^I = \bar{a}_\lambda^I c,\quad \text{where } \bar{a}_\lambda^I = \frac{J_\omega^{\mathrm{atm}}}{\Delta\omega_{\mathrm{ef}}^{\mathrm{atm}}}\frac{\rho}{\rho^I_{\mathrm{atm}}} \tag{5}$$

Here ρ^I_{atm} is the density of water impurity at atmospheric pressure. In the glass medium water molecules are located far from each other and thus can be treated independently. In that case radiation is also scattered independently by separate molecules and the phase function for the examined medium is the same as for a single molecule. Water molecules are scattering objects with a small size parameter and scattering by these particles may be represented by a linear anisotropic phase function in the form [9]

$$\Phi(\nu_i,\nu) = 1 + b\nu_i\nu$$

where parameter b is asymmetry factor whose values lie between −1 and 1. Particular cases of b equal to −1, 0, and 1 correspond to backward, isotropic, and forward scattering, respectively.

Now let us specify the effect of radiation in terms of heat sources per unit mass of matrix and water impurity due to absorption of radiation. They are obtained by multiplying spectral intensity of radiation by appropriate spectral absorption coefficient and integrating the product over solid angle and wavelength and appear as

$$Q^M(\bar{z}, c) = \frac{2\pi}{\rho^M} \int_0^\infty a_\lambda^M \left(\int_{-1}^{1} I_\lambda(\bar{z}, \nu, c)\, \mathrm{d}\nu \right) \mathrm{d}\lambda$$

$$Q^I(\bar{z}, c) = \frac{2\pi}{\rho^I} \sum_{k=1}^{P} \int_0^\infty a_{\lambda_k}^I(c) \left(\int_{-1}^{1} I_\lambda(\bar{z}, \nu, c)\, \mathrm{d}\nu \right) \mathrm{d}\lambda \tag{6}$$

Then the total heat sources in the layer are

$$Q = Q^M + Q^I \tag{7}$$

Since the glass matrix absorbs radiation in the entire range of spectrum, while water impurity does that in narrow bands, in the entire spectrum range two kinds of intervals can be distinguished, namely those where just matrix absorbs and those where both matrix and water absorb. By accounting for that in Eq. (6) we obtain

$$Q^M(\bar{z}, c) = \frac{2\pi}{\rho^M} \sum_{k=0}^{P} \left(\int_{\lambda_{k,r}}^{\lambda_{k+1,l}} a_\lambda^M \bar{I}_\lambda \, \mathrm{d}\lambda + \int_{\lambda_{k+1,l}}^{\lambda_{k+1,r}} a_\lambda^M \bar{I}_\lambda \, \mathrm{d}\lambda \right)$$

$$Q^I(\bar{z}, c) = \frac{2\pi}{\rho^I} \sum_{k=1}^{P} \int_{\lambda_{k,l}}^{\lambda_{k,r}} a_{\lambda_k}^I(c) \bar{I}_\lambda \, \mathrm{d}\lambda$$

$$\bar{I}_\lambda = \int_{-1}^{1} I_\lambda(\bar{z}, \nu, c)\, \mathrm{d}\lambda \tag{8}$$

Here $\lambda_{k,l}$ and $\lambda_{k,r}$ are left and right edges of the kth band respectively ($\lambda_{k,r} - \lambda_{k,l} = \Delta\lambda_{\mathrm{ef}}^k$ where $\Delta\lambda_{\mathrm{ef}}^k$ is the effective width of the kth band in terms of wavelength), $\lambda_{0,r} = 0$; $\lambda_{P+1,l} = \lambda_{P+1,r} = \infty$. In the spectrum ranges $\lambda_{k,r} < \lambda < \lambda_{k+1,l}$, $k = 0, 1, \ldots, P$, where just glass matrix absorbs, the spectral intensity of radiation $\bar{I}_\lambda$ becomes a function of $\bar{z}$ and ν only. The spectral intervals of water impurity absorption and scattering are assumed to coincide.

3. Governing equations

The set of governing equations of the model consists of the transient energy equation for the entire medium and the water impurity diffusion equation, supplemented by appropriate boundary conditions. Effect of radiation is taken into account in these equations by total heat sources Q present in the transient energy equation and implicitly by quantity E^I, which is a function of Q^I, in the impurity diffusion equation [7]. The transient energy equation and the water impurity diffusion equation appear as follows

$$\rho C \frac{\partial T}{\partial t} = \chi \frac{\partial^2 T}{\partial z^2} + \rho Q, \qquad \frac{\partial c}{\partial t} = \frac{\partial}{\partial z} \left(D(E^I) \frac{\partial c}{\partial z} \right)$$

Introducing in these equations corresponding dimensionless times $\tau_T = \kappa t / h^2$ and $\tau_c = D_0 t / h^2$ (κ is the thermal diffusivity), we obtain the following equations

$$\frac{\partial T}{\partial \tau_T} = \frac{\partial^2 T}{\partial \bar{z}^2} + \frac{h^2}{\chi} \rho Q \tag{9}$$

$$\frac{\partial c}{\partial \tau_c} = \frac{\partial}{\partial \bar{z}} \left(\frac{D(E^I)}{D_0} \frac{\partial c}{\partial \bar{z}} \right) \tag{10}$$

Here diffusivity $D(E^I)$ is defined by the expression [7,8]

$$D(E^I) = D_0 \exp(-E_{\mathrm{act}} / E^I).$$

Quantity E^I is introduced in the model in order to capture the effect of selective absorption of radiation by water impurity. The value of E^I is balanced by absorption of radiation and energy dissipation on thermal vibrations of the matrix [7]. In the considered glass medium the water phase is in the form of separate molecules. Therefore, macroscopic considerations cannot be involved in determining water phase temperature, as it was done for the aluminium phase in a solid composite in [6]. Indeed, individual molecules do not possess physical characteristics proper for their agglomeration. To overcome this difficulty, the method to determine E^I approximately was proposed in [8]. Omitting technicalities given there, we arrive at the following equation for the determination of E^I

$$E^I = \frac{2}{3} M^I Q^I t + \overline{R} T_0 \leqslant E_{\max}^I, \quad \text{if } L(z) \geqslant 1 \tag{11a}$$

$$E^I = \overline{R} T, \quad \text{if } L(z) < 1 \tag{11b}$$

Here T_0 is the initial temperature. Parameter L was introduced in the model [7] to determine the prevailing way of energy exchange for the impurity. This is a complex parameter dependent on characteristics of the radiation intensity and parameters of impurity diffusion. If $L \geqslant 1$ it means that the rate of absorption of radiation energy by impurity is much higher than the rate of its energy dissipation on the glass matrix and the thermal state of the impurity is determined by its energy $E^I \geqslant \overline{R} T$ (the heating of impurity according to Eq. (11a) lasts until E^I reaches its maximum value $E_{\max}^I$). The case of $L < 1$ corresponds to the situation where there is no specific effect of radiation on impurity and its thermal state is the same as of the entire medium, namely $E^I = \overline{R} T$.

At the boundaries of the layer the following heat and mass exchange conditions are taken

$$\begin{aligned} &\frac{\partial T(0)}{\partial \bar{z}} - Bi_T \big(T(0) - T_a \big) = 0 \\ &\frac{\partial T(1)}{\partial \bar{z}} + Bi_T \big(T(1) - T_a \big) = 0 \end{aligned} \tag{12}$$

$$\begin{aligned} &\mathrm{J}(0) - Bi_c \big(c(0) - c_s \big) = 0 \\ &\mathrm{J}(1) + Bi_c \big(c(1) - c_s \big) = 0 \end{aligned} \tag{13}$$

where J is the mass flux in the direction normal to axis z, T_a is the ambient temperature, c_s is the impurity concentration in surroundings. Therefore, together with initial conditions

$$T(\bar{z})|_{t=0} = T_0(\bar{z}) \tag{14}$$

$$c(\bar{z})|_{t=0} = c_0(\bar{z}) \tag{15}$$

they complete the formulation of the model equations consisting of the radiation transfer equations (1)–(2), the transient energy equation (9), the water impurity diffusion equation (10), the equation for determining impurity molar energy E^I (11), the heat and mass exchange boundary conditions (12), (13) and initial conditions (14), (15).

4. Numerical procedure

The system of model equations (1), (9)–(11) together with corresponding boundary conditions (2), (12)–(15) was solved by an iterative method. As an initial approximation, the solution of model equations obtained at the values of spectral absorption coefficient a_λ, diffusion coefficient of impurity D and impurity molar energy E^I, calculated at initial distributions of the impurity concentration and the temperature is taken. For each time moment, on a particular iteration the radiation transfer equation is solved first. The spectral intensity of radiation is found, the total heat sources Q and heat sources in water impurity Q^I are computed. These quantities are then substituted into the transient energy equation and the impurity diffusion equation. Found temperature and concentration of the impurity are then used in the radiation transfer equation to compute updated spectral intensity of radiation. Iterations are halted when the predetermined accuracy is reached.

On a particular iterations, the radiation transfer equation was solved by the discrete ordinates method while for solving the transient energy equation and the impurity diffusion equation the finite difference method was applied. In solving the latter equations a fully implicit time-marching technique was used. To obtain solution to the radiation transfer equation by the discrete ordinate method we used the results presented in Fiveland's work [9]. In doing so, the radiation transfer equation (1) in a given spatial point is split in a set of N equations written for a discrete number of ordinate directions N and the integrals are replaced by a numerical quadrature in each of these equations to appear as

$$\nu_n \frac{\partial I_n}{\partial \theta} = -I_n + \frac{\Omega}{2} \sum_{n'=1}^{N} I_{n'} \Phi_{nn'} w_{n'}, \quad n' = 1, 2, \ldots, N \tag{16}$$

Here $w_{n'}$ are weights of the quadrature; subscript λ, denoting spectral quantity, is omitted here and further on for the sake of simplicity. In a similar manner boundary conditions (2) are written as

$$\begin{aligned} &I_n(0) = I_n(0) + 2R \sum_{n'=1;\, \nu_{n'}<0}^{N} I_{n'} \nu_{n'} w_{n'} \\ &\quad z = 0,\ n' = 1, 2, \ldots, N \\ &I_n(1) = I_n(1) + 2R \sum_{n'=1;\, \nu_{n'}>0}^{N} I_{n'} \nu_{n'} w_{n'} \\ &\quad z = 1,\ n' = 1, 2, \ldots, N \end{aligned} \tag{17}$$

A number of numerical quadratures were proposed for the discrete ordinate method. In this study S–N quadrature weights and points were taken as proven to be sufficiently accurate for the one-dimensional case [9]. In particular, in this paper S–N quadrature weights are used, which were constructed in [9] in the way to satisfy the first moment of radiation intensity over half range (surfacial radiation flux) what is important in combined heat transfer mode problems.

To relate intensities in neighbouring points of spatial grid different spatial differencing schemes were proposed for 2D and 3D problems [14]. In the examined here one-dimensional case, intensities are coupled by using a simple difference form to appear as follows for positive ordinate directions [9]

$$I_{j+1}^n = \frac{(\nu_n/l - 1/2) I_j^n + \frac{\Omega}{2} \sum_{n'=1}^{N} I_j^{n'} \Phi_{nn'} w_{n'}}{(\nu_n/l + 1/2)} \tag{18}$$

and in a similar form for negative ordinate directions. Here $l = (a + \sigma)h/M$, where M is the number of spatial points. Solution procedure for each of n directions is iterative since intensities in Eq. (18) are coupled on both spatial and angular grids. Computations begin by assuming nonreflective boundaries and zero in-scattering terms. On marching in both positive and negative ordinate directions the spectral intensities I_j^n $(j = 1, 2, \ldots, M,\ n = 1, 2, \ldots, N)$ are found. On subsequent iterations real boundary conditions and in-scattering terms are involved. Iterations take place until a pre-determined accuracy of radiation intensity values is reached.

Two issues, treated as drawbacks of discrete ordinates method, are often discussed by the researchers, namely the ray effect and false scattering. These drawbacks are attributed to angular and spatial discretisations, respectively [15]. The ray effect is associated with the situation when some walls in 2D or 3D enclosure are unseen by the beam while from the physical consideration of the problem it appears to be impossible. It is usually the case when just a small strip on one of the walls emits. The one-dimensional problem examined here is free of ray effect because each ray emitted by the boundary of the layer reachs the opposite boundary, except for those completely attenuated. False scattering is associated with the case when radiation falsely propagates in some directions though it is known to be impossible. Again, false scattering is related to a particular situation when small parts of the wall emit and thus it does not concern the case examined here.

5. Computational experiments

Calculations were carried out for a 1 cm thick layer. Only boundary $z = 0$ of the layer was irradiated. Schematics of the model is presented in Fig. 1. The medium separating the radiation source and the layer was assumed to be transparent. In all cases initial temperature and water impurity concentration in the layer were assumed uniform.

In our computations fused silica glass as a material of the layer was chosen. Its spectral absorption coefficient is given as follows [16]

$$a_\lambda^M = a_1, \quad 0.2 \leqslant \lambda \leqslant 2.8\ \mu\text{m}$$
$$a_\lambda^M = a_2, \quad 2.8 \leqslant \lambda \leqslant 4.8\ \mu\text{m}$$
$$a_\lambda^M = a_3, \quad 4.8 < \lambda\ \mu\text{m}$$

It was shown recently [16] that accounting for absorption in the range $0.2 \leqslant \lambda \leqslant 2.8$ µm is important for the accurate prediction of the temperature field in the fiber drawing process, despite low values of the absorption coefficient in this range. Five bands model for water absorption [13] was considered here.

5.1. Effect of scattering

Water heat sources distributions in the cases of pure absorption and absorption and scattering are compared in Fig. 2. In the case we are interested in here accounting for scattering brings little changes to heat sources in the water impurity. In particular, heat sources are higher when accounting for scattering compared to the pure absorption case, near irradiated boundary of the layer. In the case of scattering some extra amount of radiation is reflected by the boundary thus increasing the value of radiation intensity to be absorbed in the vicinity of the boundary of the layer.

The effect of scattering on water diffusion was also examined. Since diffusion is a very slow process, considered above little changes in heat sources in water brought by accounting for scattering translate to insignificant changes in diffusion. However, a general tendency is observed that the higher the scattering coefficient is, the slower is diffusion. For example, after 8 hours of radiation action the total mass of water released from the layer due to diffusion is 2.8% in the case of pure absorption and 2.6% in the case of absorption and scattering. Although the effect of scattering on water diffusion is small, general considerations within the model suggest that this effect can be more pronounced for impurities with higher diffusion activation energy irradiated by relatively low intensities. Under those conditions it would take more time for Q^I to get their steady values. As those values are reached the thermal state of impurity no longer depends on radiation intensity and, therefore, on partial contributions of absorption and scattering.

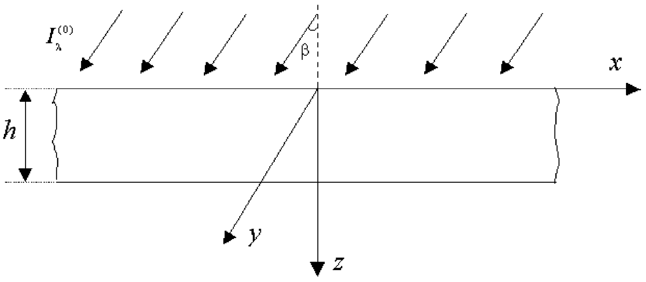

Fig. 1. Schematics of the model.

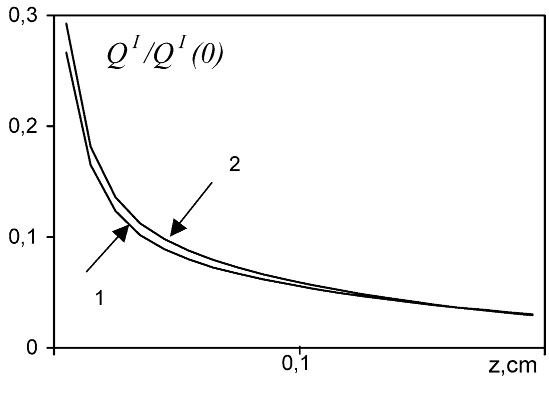

Fig. 2. Dimensionless water heat sources in the case of pure absorption (1) and absorption and scattering (2).

5.2. Effect of water impurity on the temperature field

The water content in glasses may vary in a very wide range [5,16] so that investigations of temperature distributions at different values of water concentrations in the layer are carried out. It is established that the presence of water influences the temperature field and the effect is maximum at certain value of water concentration. In Fig. 3 temperature distributions over the thickness of the layer are presented for three different values of water concentration. Curve 2 corresponds to the case where layer is, in fact, free of water ($c_0 = 10^{-8}$). Increase in the water concentration causes a temperature rise. The maximum value of concentration in this case is $c_0 = 10^{-3}$ (curve 1). Further increase of water concentration, however, does not lead to continuing temperature rise. Moreover, temperature decreases, and at water concentration equal to 0.1 (curve 3) the temperature field in the layer practically coincides with that in the water free layer. This temperature behavior can be explained analyzing distributions of heat sources in water, Q^I, plotted in Fig. 4. In the case of $c_0 = 10^{-3}$ water concentration is high enough to absorb radiation in the amount making a noticeable effect on the temperature in the layer, while allowing a substan-

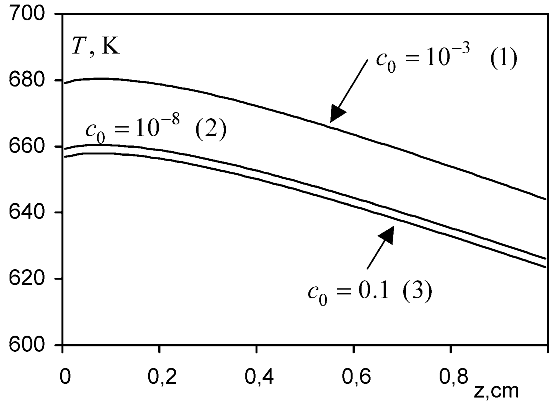

Fig. 3. Steady-state temperature distributions at different water impurity concentrations.

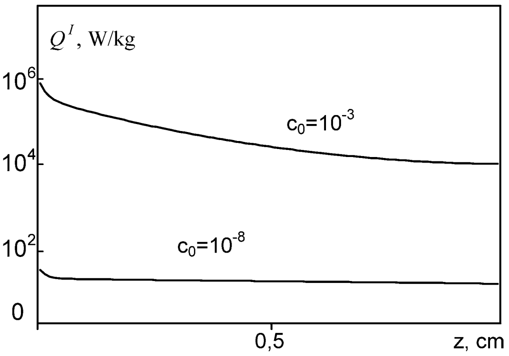

Fig. 4. Water heat sources at different concentrations.

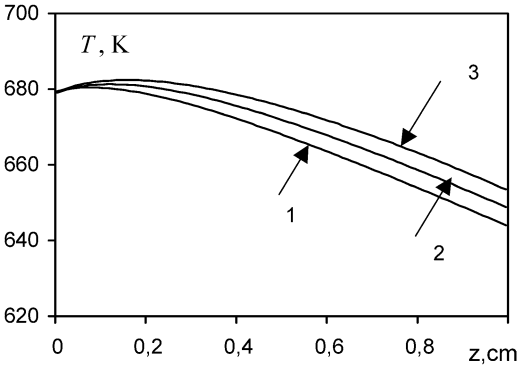

Fig. 5. Steady-state temperature distributions at different spectral content of radiation. (1) $T_S = 3000$ K; (2) $T_S = 2000$ K; (3) $T_S = 1500$ K.)

tial portion of radiation to get inside the layer. When water concentration is 10^{-8} heat sources are almost uniformly distributed over the thickness of the layer. However, they are too small to produce any significant effect on the temperature in the layer. When water is present in the layer with concentration 0.1, its heat sources become surfacial ones (not shown) due to very strong absorption, therefore producing a negligible effect on the temperature of the layer.

In Fig. 5 the effect of the temperature of thermal radiation source on the temperature distributions in the impurity free layer is demonstrated. Coefficient $k^{(0)}$ in expression (3) for each radiation source temperature is selected in such a way that it provides the same level of maximum temperature in the layer. Curves 1–3 correspond to radiation source temperatures 3000, 2000, and 1500 K, respectively. In can be concluded from Fig. 5 that the radiation intensity shift to shorter wavelengths results in reducing temperature gradients in the layer. This can be attributed to the fact that fused silica glass is essentially transparent in the range $0.2 \leqslant \lambda \leqslant 2.8$ µm.

6. Conclusions

In this study we have examined the effect of the presence of molecular water impurity in the fused silica glass on the temperature field in the layer subjected to thermal infrared radiation. Radiation absorption and scattering were taken into account in the developed model. It was established that the presence of water impurity may influence significantly on the temperature distribution in the layer. This effect grows with increasing water concentrations and has its maximum impact at certain value of water concentration. Further increase of water concentration, however, leads to a decrease of this impact. In particular, at the maximum possible value of water concentration this effect is practically negligible which can be attributed to water becoming opaque at this concentration. It has been shown that the radiation intensity shift to shorter wavelengths range produces smaller temperature gradients in the layer.

We have also analysed the effect of scattering on thermal and diffusive processes in the considered medium. Scattering makes heat sources in the water more nonuniform over the thickness of the layer. However, the resultant temperature field is not affected since water impurity heat sources represent a small part of the total heat sources in the glass. Effect of scattering on diffusion is generally insignificant, though diffusion tends to be slower with larger scattering coefficient.

One of the important results of the present model is that an external radiation provides selective effect on individual constituent of multicomponent semitransparent solid resulting in specific value of impurity diffusion coefficient and promotion of impurity diffusion. This agrees well with the experimental results presented in [4,5] where obtaining of composite (i.e., multicomponent) materials with improved mechanical properties was explained by individual response of different constituent to external microwave radiation leading to enhanced diffusion of certain constituent. In this sense, the model developed here may be treated as an attempt to give theoretical description of selective effect of radiation on multicomponent materials.

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