About control of convection intensity in chemical active equilibrium gas

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Abstract

The problem of the Rayleigh-Benard convection for a chemical equilibrium gas is investigated using methods of linear analysis. The Boussinesq approximation is used for a plane layer with isothermal horizontal boundaries free from shearing stresses. A previously developed model for chemical equilibrium is applied to calculate the thermodynamic parameters of the gas analyzed (hydrogen-oxygen mixture). Recombination and dissociation processes are shown to introduce an additional factor multiplying the Rayleigh number defined as in inert gas. Formulas for the increment of growth o infinitesimal perturbation and the critical Rayleigh number as a function of absolute temperature are obtained.

Key words: Rayleigh-Benard convection, Rayleigh number, Prandtl number, chemical equilibrium, recombination, dissociation.

Introduction

The Rayleigh-Benard convection is a type of natural convection belonging to the area of classic science in whose frameworks a mathematical model based on the Boussinesq approximation and numeric methods were developed for this convection [1-4,13]. Scientists mainly focused on modelling convection for chemically inert gases and liquids.

Convection processes happen in chemically reacting media as well. Such type of convection can be observed while gas mixture burns in large-scale reactors, technical installations and experimental facilities.

Convection of a gas in chemical equilibrium is a particular, though quite common, case of convection in gases accompanied by chemical reactions, which can occur if the time scale of the reaction is much shorter than that characteristic for the convection process.

It should be expected that quantitative and qualitative characteristics of convection mainly depend on the type of the thermal expansion coefficient dependence on temperature, which determines the buoyancy force casing convection.

The thermal expansion coefficient of a chemically inert gas is monotonic and inversely related to the temperature. In the case of a chemically active equilibrium gas, the dependence of this coefficient on temperature changes considerably and becomes non-monotonic with a clear local maximum, where the value of the coefficient for a chemical equilibrium gas can exceed that of a chemically inert gas by several times [5-9]. Such anomalous dependence of the coefficient on the temperature expansion (other than $1/T$) leads to considerable changes in quantitative and qualitative characteristics of convection regimes in a chemical equilibrium gas compared to those in a chemically inert gas.

Authors in [10-12] were the first to formulate and solve numerically a two-dimensional problem for Rayleigh-Benard convection in a chemically active equilibrium gas, as well as considered linear and non-linear regimes. The molar mass and thermodynamic parameters of the gas were calculated according to a previously developed model of chemical equilibrium [5-9]. The results of the linear and non-linear analysis [10-12] need additional investigations and improvements. In addition, the physical and mathematical model provided in [10-12] is quite complicated and inconvenient; while representing the dependence of the thermal expansion coefficient on the whole range of the real (not dimensionless!) temperature, a second degree polynomial equation with four constants is used instead.

Further investigations into the problem showed that the realization of the model proposed in [10-12] can be considerably simplified as recombination and dissociation processes in gases under the temperature given can be taken into account through multiplying the Rayleigh number by an additional factor, the function of absolute temperature.

In terms of convection in a laboratory, the gas compressibility can be neglected and the convection media can be considered as incompressible. Moreover, if the domain has a certain geometry and small supercriticality, convection develops as two-dimensional rollers [13], which allows us to consider two-dimensional convective flows of a viscous incompressible fluid even at the first stage of our investigation.

Following [10-12], we consider a convective two-dimensional and non-stationary flow of a viscous incompressible fluid in the horizontal layer heated from below in the Boussinesq approximation. The boundaries of the layer are assumed isothermal and free from shearing stresses. Thermodynamic parameters of a chemical equilibrium gas are calculated according to the model in [5-9].

The present work is aimed at describing a simpler and improved realization of a physical and mathematical model for convection of a chemically active gas in equilibrium and at specifying the results of the linear analysis.

Nomenclature

The following notations will be used:

ρ, P, T *and* μ - the density, pressure, absolute temperature and molar mass of the gas;
R - the universal gas constant;
μ_{min}, μ_{max} - the molar masses of the gas in the completely dissociated and completely recombined states;
A, K_+ - the rate constants of dissociation and recombination of the generalized reaction products;
θ - the effective excitation temperature of the vibrational degrees of freedom of the molecules;
E - the mean dissociation energy of the reaction products;
β - the thermal expansion coefficient of the gas with chemical reactions;
$\beta_{in} = 1/T$ - the thermal expansion coefficient of the inert ideal gas;
u, v - the velocities in x and y directions;
ν, χ - the kinematic and thermal diffusivity coefficients;
T_h, T_c - the temperatures of the lower and upper boundaries;
H - the thickness of the layer;
ψ - the stream function ($\psi_y = u$ and $\psi_x = -v$);
ω - the vorticity $\omega = v_x - u_y$;
$Ra = g\beta H^3 \delta T/\chi\nu$ - Rayleigh number;
Ra_{cr}, α_m - the critical values of Rayleigh and wave numbers;
$Pr = \nu/\chi$ - Prandtl number;
$\lambda, \alpha, \pi m$ - the eigenvalue and the wavenumbers of linear problem in x and y directions;
$Q = T-T_e$ - the temperature deviation from linear equilibrium distribution.

Kinetic model

To describe chemical equilibrium in the gas mixture, we use a highly accurate kinetic model [5-9]. According to this approach, the density of a chemical equilibrium ideal gas can be considered as a function of the absolute temperature and pressure:

$$\rho = \frac{p\mu}{RT},$$

$$\mu = \frac{B\mu_{\min} - 2\mu_{\max} + ((B\mu_{\min} - 2\mu_{\max})^2 + 4(B-1)\mu_{\max}^2)^{0.5}}{2(B-1)}, \qquad (1)$$

$$B = \frac{AT^{0.75}}{4K_+} \cdot (1 - \exp(-\Theta/T))^{1.5} \exp(-E/RT)) \frac{\mu_{\max}^2}{\mu_{\min}\rho}.$$

The molar mass of the gas can vary within the interval $\mu_{min} \le \mu \le \mu_{max}$. We have $\mu \to \mu_{max}$ with decreasing temperature and $\mu \to \mu_{min}$ with increasing temperature.

We assume that the pressure P in the gas mixture (external pressure) is constant. Then, the gas density ρ, as is seen from system (1), depends on the absolute temperature T only. For the purposes of comparing our results with those in [10-12], our linear analysis was performed with the pressure changing in the same range, from 10^{-5}atm to 10^5atm.

The model of chemical equilibrium used [5-9] favors simplicity, accuracy and compatibility with the principle of entropy increase. It takes into account considerable changes of the molar mass, the temperature effect, heat capacities and the ratio of specific heats due to the change of chemical equilibrium. All the constants in the model are physically clear.

Such equations are usually used to calculate chemical equilibrium in hydrogen-oxygen mixture and hydrocarbon-oxygen mixtures [6-8], in heterogeneous mixtures of gas-condensed-phase type in the presence of the interphase mass transfer [7] and heterogeneous mixtures of gases with chemically inert particles [9]. Two-stage models of detonation combustion of methane in oxygen and air have also been proposed [14].

The model of chemical equilibrium in question is particularly useful for scientific and applied problems, e.g., while modelling detonation processes in chemically active bubble systems [14,15], designing equipment for fluidized bed coating by means of gaseous detonation [16], using detonation suppression by inert particles [17-19], calculating concentration limits for gas mixture flammability [20].

As it is seen from system (1), the ratio for the molar mass as a function of temperature is as follows:

$$\mu(T) = \mu_{\max} + 0.5 \cdot (f - \sqrt{f^2 + 4f(\mu_{\max} - \mu_{\min})}),$$

$$f = \frac{AR\mu_{\max}^2 T^{1.75}}{4K_+ P\mu_{\min}} \cdot (1 - \exp(-\Theta/T))^{1.5} \exp(-E/RT)).$$

The present paper refers to a stoichiometric hydrogen-oxygen mixture. The numerical values of the constants were as follow: $E = 459.2 \cdot kJ/mole$, $\Theta = 4000K$, $K_+ = 6 \cdot 10^8 m^6/(kmole^2 \cdot sec)$, $A = 5.1 \cdot 10^{10} m^3/(kmole \cdot sec \cdot K^{3/4})$, $\mu_{min} = 6kg/kmole$, $\mu_{max} = 18kg/kmole$ [5-9].

Considering the ratio for f at comparatively “low” and high temperatures T and taking into account

$$f \,\square\, T^{1.75} \cdot \exp(-\frac{E}{RT}) \,\square\, \exp(-\frac{E}{RT}) \;\; (T \,\square\, \Theta), \;\; f \,\square\, T^{0.25} \; (E/R \,\square\, T),$$

we have the following for the “low” temperature

$$T \to 0, \;\; f \to 0, \;\; \mu_{as1} = \mu_{\max} - f^{0.5}(\mu_{\max} - \mu_{\min})^{0.5} + f/2 + O(f^{3/2})$$

and for the high temperature

$$T \to \infty,\ f \to \infty,\ \mu_{as2} = \mu_{\min} + (\mu_{\max} - \mu_{\min})^2 / f + O(f^{-2}).$$

The thermal expansion coefficient β can be found dependent on the density or the molar mass as

$$\beta = -\frac{1}{\rho} \cdot \frac{\partial \rho}{\partial T} = -\frac{d}{dT} \ln(\mu / T) = \frac{1}{T} - \frac{1}{\mu} \frac{d\mu}{dT}.$$

Notice that the asymptotic approximation of the molar mass μ to constants as the temperature is reduced or increased allows us to find the asymptotics for the thermal expansion coefficient β as $\beta = 1/T$.

Figures 1-4 and 7 show the asymptotic curves calculated with the full formula for f where all the coefficients in expression for f were used. Figures 1 - 7 were plotted with $P = 1atm$.

The solid curve in Fig. 1 shows the molar mass $\mu = \mu\ (T)$, asymptotics for the “low” ($\mu_{as}1$, curve 1) and high ($\mu_{as}2$, curve 2) temperatures as well as $\mu = \mu_{max}\ (3)$ and $\mu = \mu_{min}\ (4)$. The asymptotic curves $\mu_{as}1$ (curve 1) and $\mu_{as}2$ (curve 2) are correct for both comparatively low ($T \le 3500K$) and high ($T \ge 5000K$) temperatures.

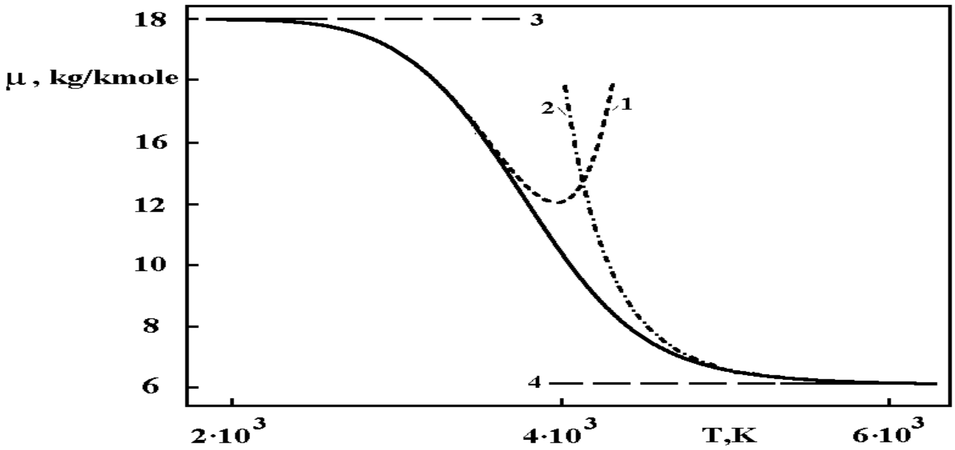

Fig. 1. The molar mass and its asymptotics

The solid curve in Fig. 2 shows the density of the chemical equilibrium gas $\rho = \rho(T)$ at $2{\cdot}10^3K \le T \le 6{\cdot}10^3K$. Again, we see two asymptotics $\rho_1 = \mu_{as1}P/(RT)$ (dashed curve 1) and $\rho_2 = \mu_{as2}P/(RT)$ (dashed curve 2) corresponding to comparatively low ($T \le 3500K$) and high ($T \ge 5000K$) temperatures, in comparison to curves $\rho_3 = \mu_{max}P/(RT)$ (dot-and-dash curve 3) and $\rho_4 = \mu_{min}P/(RT)$ (dot-and-dash curve 4) for absolutely recombined and dissociated conditions respectively. The curves are quite accurate for both low and high temperatures. Notice that throughout the range of temperature changes the density depends on the temperature monotonically.

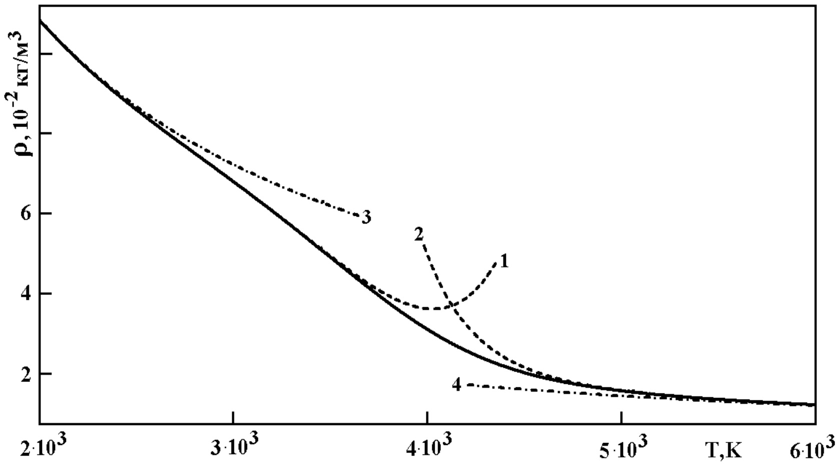

Fig. 2. The gas density

The solid curve in Fig. 3 shows the thermal expansion coefficient $\beta = \beta(T)$ while the dot-and-dash line $\beta = 1/T$ for ideal gas shows the close values at $T \le 2000K$ and $T \ge 6000K$. Again, we see two asymptotics (dashed curves 1 and 2) with close values at comparatively low ($T \le 3500K$) and high ($T \ge 5000K$) temperatures. We see the temperature interval where the thermal expansion coefficient β demonstrates an anomalous behavior (different from $1/T$) with noticeable local maximum. As it is shown below, it is this anomalous behavior that causes a possibility of convective instability amplification in comparison with inert gas.

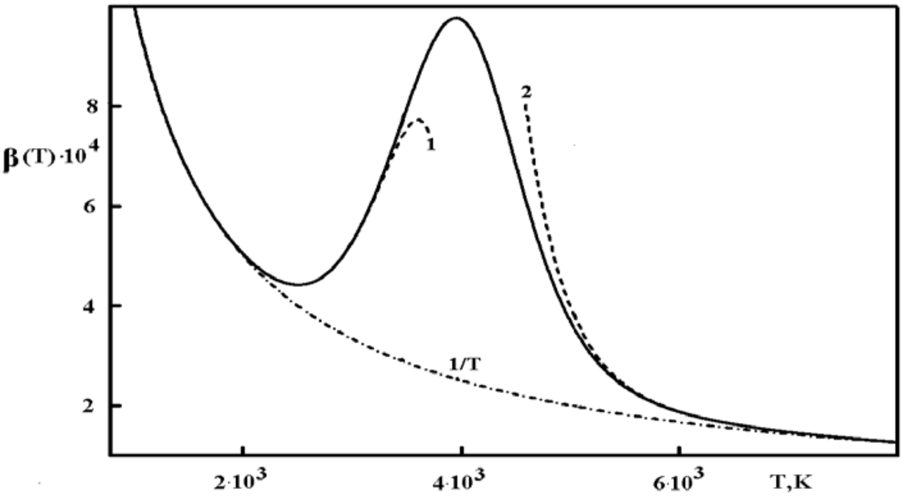

Fig.3. The thermal expansion coefficient

Mathematical model

Convection of incompressible fluids in the Boussinesq approximation is described by the following system of equations [1,2]:

$$
\begin{aligned}
&\omega_t + \frac{1}{\Pr}(\psi_y \omega_x - \psi_x \omega_y) = \Delta\omega + C \cdot Ra \mathrm{Q}_x, \\
&\Delta\psi = -\omega, \\
&\mathrm{Q}_t + \frac{1}{\Pr}(\psi_y \mathrm{Q}_x - \psi_x \mathrm{Q}_y) = \frac{1}{\Pr}\Delta\mathrm{Q} - \frac{1}{\Pr}\psi_x, \qquad (2) \\
&C = \frac{\beta(T)}{\beta_{in}(T)} = T \cdot \beta(T).
\end{aligned}
$$

Here, $Ra = g\beta_{in}H^3\delta T/\chi\nu = gH^3\delta T/(T\chi\nu)$ and $Pr = \nu/\chi$ are Rayleigh and Prandtl numbers, here $\beta_{in} = 1/T$ is the thermal expansion coefficient of the inert ideal gas as function of the absolute temperature T.

We choose the following reference values for the layer: H for length, H^2/ν for time, χ/H for velocity, $\rho_0\nu\chi/H^2$ for pressure, $\rho_0 = \rho(T)$ for density, and $\delta T = T_h - T_c$ for temperature, Q is temperature deviation from equilibrium linear distribution, $\Delta f = f_{xx} + f_{yy}$ is the Laplace operator, φ and ω are stream function and vorticity respectively. The thermal expansion coefficient β is considering as constant in system (2) at chosen absolute temperature T.

According to the buoyancy force in the first equation of system (2), we see that the convection rate is defined by $C{\cdot}Ra$. The Rayleigh criterion specifies the ratio between the buoyancy force and the viscosity and depends on the temperature gradient or the degree of heating, while the dimensionless factor C depends on the recombination and dissociation processes under the temperature given.

Figure 4 shows function $C = C(T)$ at $P = 1atm$ and two asymptotes (dashed curves 1 and 2). It can be seen that in domain ($2000K \le T \le 8000K$) the chemical reactions in gas increase the convection intensity. When the temperature falls ($T < 2000K$) or rises ($T > 8000K$), the convection intensity decreases up to convection intensity level in an ideal inert gas. The maximum convection intensity is realized at the points of local extremum of the factor $C = 3.907$ at $T = 4051K$.

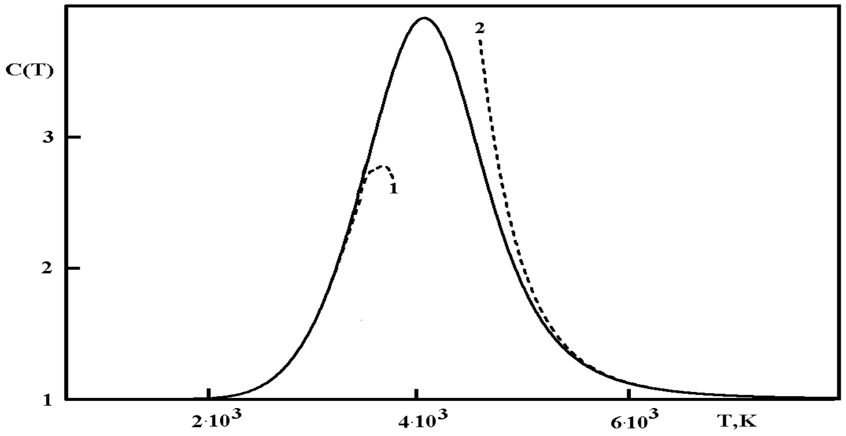

Fig. 4. Factor $C = C(T)$

Considering the relation for f at comparatively “low” and high absolute temperatures T, we have the following asymptotics for the “low” and high temperature

$$
fas1 = \frac{AR\mu_{\max}^2 T^{1.75}}{4K_+P\mu_{\min}} \cdot \exp(-E/RT)) \quad (T \square \Theta),
$$

$$
fas2 = \frac{AR\mu_{\max}^2 T^{0.25}\Theta^{1.5}}{4K_+P\mu_{\min}} \quad (E/R \square T).
$$

The solid curve in Fig. 5 shows the function $f = f(T)$ and its two asymptotes fas1 and fas2 (dashed curves 1 and 2) with close values at comparatively "low" ($T \leq 4000K$) and high ($T \geq 55000K$) temperatures. The two vertical lines correspond $T = \Theta = 4000K$ and $T = E/R = 5.523 \cdot 10^4$.

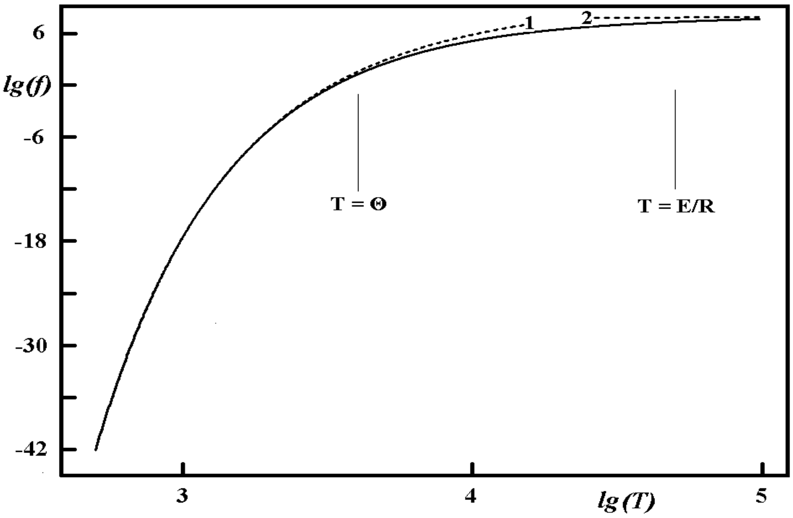

Fig. 5. The function *f(T)*

At a considerably high temperature ($T \sim E/R \sim 5 \cdot 10^4 K$) power asymptotics for f is stated, which allows us to obtain far-field asymptotics for β and C.
Actually, taking into account

$$f \to fas2 = \frac{AR\mu_{\max}^2\Theta^{1.5}}{4K_+P\mu_{\min}}T^{0.25} \ (T \to \infty),$$

we find $\beta = \frac{1}{T}(1 + \frac{(\mu_{\max} - \mu_{\min})^2 K_+ P}{AR\mu_{\max}^2\Theta^{1.5}}\frac{1}{T^{0.25}}), \quad C = 1 + \frac{(\mu_{\max} - \mu_{\min})^2 K_+ P}{AR\mu_{\max}^2\Theta^{1.5}}\frac{1}{T^{0.25}}$.

The dependences given show that β and C approach asymptotics with the rise of the temperature quite slowly, which means that the corresponding boundary is fuzzy.

Linear analysis

We consider the linear analog of system (2):

$$\begin{aligned} \omega_t &= \Delta\omega + C \cdot Ra\mathrm{Q}_x, \\ \Delta\psi &= -\omega, \\ \mathrm{Q}_t &= \frac{1}{\mathrm{Pr}}\Delta\mathrm{Q} - \frac{1}{\mathrm{Pr}}\psi_x. \end{aligned} \tag{3}$$

We seek approximate solutions of system (3) in the form:

$$\begin{aligned} \omega(t,x,y) &= \Omega\exp(-\lambda t)\cos(\alpha x)\sin(m\pi y), \\ \psi(t,x,y) &= \Omega\exp(-\lambda t)\cos(\alpha x)\sin(m\pi y)/S, \\ \mathrm{Q}(t,x,y) &= \Theta\exp(-\lambda t)\cos(\alpha x)\sin(m\pi y), \\ S &= \alpha^2 + m^2\pi^2. \end{aligned} \tag{4}$$

Here λ is the eigenvalue, where $\lambda > 0$ is matched by amplitude losses and $\lambda < 0$ by amplitude rises in harmonic solutions, α and $m\pi$ are the wavenumbers in x and y directions, and Ω and Θ are constants.

Plugging (4) into (3) and using standard calculations [1,2] we find:

$$\lambda_{1,2} = \frac{1+\Pr}{2\Pr} S \pm \sqrt{\left(\frac{1-\Pr}{2\Pr}\right)^2 S^2 + \frac{C \cdot Ra \cdot \alpha^2}{S \Pr}}, \qquad (5)$$

where $S = \alpha^2 + m^2\pi^2$, too.

Let us consider the ratio $d\lambda = \lambda_{in}/\lambda_r$ between maximal increments in the inert λ_{in} and reacting λ_r gases. The asymptotical value of $d\lambda$ can be found as

$$\frac{\lambda_{in}}{\lambda_r} \to 1/\sqrt{C\max} = 0.506 \ \ at\ Ra \to \infty.$$

Here the maximum of the factor $Cmax$ is equal to 3.907 at $P = 1atm$ *and* $T = 4051K$.

Figure 6 shows the value $d\lambda = \lambda_{in}/\lambda_r$ as function of the supercriticality $r = Ra/657.511$ where the pressure and absolute temperature are equal to 1atm and 4051K respectively. It can be seen that three distinct domains exist at various supercriticality r. At $0 < r < 1/Cmax$, $1/Cmax = 0.256$ (domain d1) only the quantitative difference is observed since the convection in inert and reacting gases is stable. At $1/Cmax \le r < 1$ (d2) the qualitative difference is seen since the convection in inert gas is stable and convection in reacting gas is unstable or neutral. At $1 \le r$ (d3) the quantitative difference is observed since the convection in the inert and reacting gases is unstable (or neutral for inert gas).

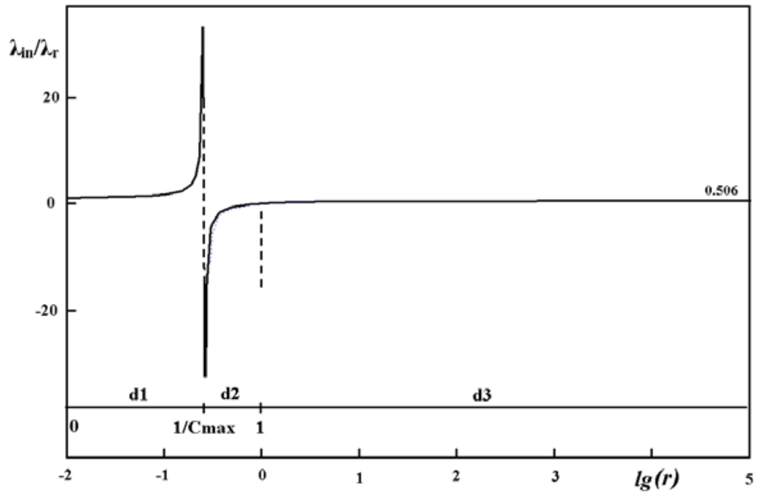

Fig.6. The increment ratio $d\lambda$ versus supercriticality r

Assuming increment λ_2 in (5) equal to 0, one can obtain the Rayleigh number corresponding to the neutral curve:

$$Ra = \frac{(m^2\pi^2 + \alpha^2)^3}{C \cdot \alpha^2}.$$

The critical value of the Rayleigh number (minimum of Ra versus α with $m = 1$) can be found by the formula

$$Ra_{cr} = \frac{27}{4C}\pi^4 = \frac{657.511}{C}, \ \ \alpha_{cr} = 2.221.$$

The factor 657.511 is identified here as the critical value of the Rayleigh number for the convection in a chemically inert media [1,2], and the factor $1/C$ as the function of temperature and pressure is due to recombination and dissociation processes.

Providing $C - 1$ is small (for $|T - \Theta| >> 1$), one can obtain the critical value of the Rayleigh number as the principal member of the power series expansion:

$$Ra_{cr} = \frac{657.511}{C} = 657.511 \cdot (2 - C).$$

Using the C asymptotics found above under the temperature approaching infinity, we can obtain the far-field asymptotics for Ra_{cr} and lengthy asymptotic formula for increment λ.
Taking into account

$$C = 1 + \frac{(\mu_{\max} - \mu_{\min})^2 K_+ P}{4AR\,\mu_{\max}^2\,\Theta^{1.5}} \frac{1}{T^{0.25}} \ (T \to \infty), \quad \text{we have}$$

$$Ra_{cr} = 657.511 \cdot (1 - \frac{(\mu_{\max} - \mu_{\min})^2 K_+ P}{4AR\,\mu_{\max}^2\,\Theta^{1.5} T^{0.25}}) \ \text{ and}$$

$$\lambda_r = \lambda_{in} \pm \frac{(\mu_{\max} - \mu_{\min})^2 K_+ P\,Ra\,\alpha^2}{4AR\,\mu_{\max}^2\,\Theta^{1.5} S^{0.5} \sqrt{(1 - \mathrm{Pr})^2 S^3 + 4Ra\,\alpha^2\,\mathrm{Pr}}} T^{-0.25}.$$

Here λ_r and λ_{in} are increments for the reacting and inert gases correspondingly.
Figure 7 shows the critical Rayleigh number as a function of T for pressure $P = 1atm$ (solid curve), two its asymptotes (dashed curves 1 and 2) and $Ra_{cr} = 657.511 \cdot (2-C)$ (dashed curve 3). It can be seen that in domain ($3000K \le T \le 5000K$, $T \approx \Theta = 4000K$) the chemical reactions in gas considerably decrease the critical Rayleigh number.

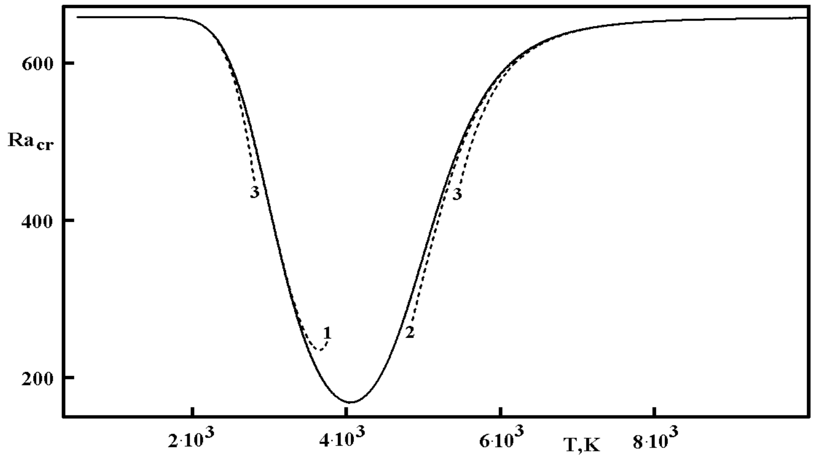

Fig.7. The neutral curve in the plane *T-Ra* for pressure 1atm

Figure 8 shows the critical Rayleigh number as a function of T for pressures $P = 1atm$ (solid curve 1), $P = 0.1atm$ (dashed curve 2), and $P = 10atm$ (dashed curve 3). The pressure increasing, the convection intensity amplification domains move while expanding towards higher temperatures. The latter is more obvious for the high-temperature boundary of domain.

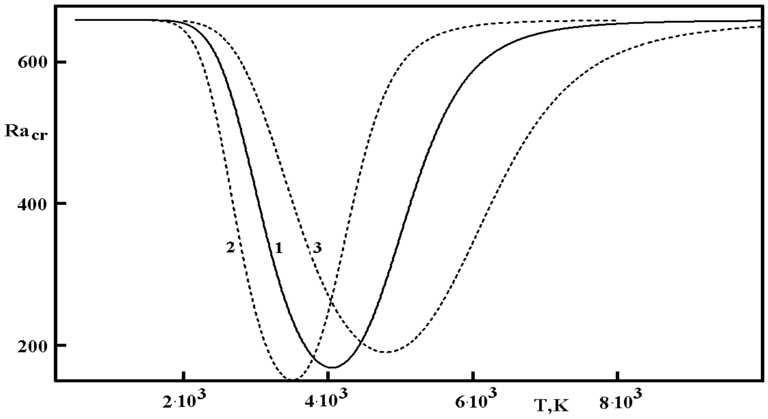

Fig.8. The neutral curve in the plane *T-Ra* for various pressure

As one can see, Figure 8 shows a relatively low increase in the critical Rayleigh number (minimum with respect to T) while the pressure increases (about 3.6 times while the pressure increases by 10 orders of magnitude):

$Ra_{cr} = 657.511/C \approx 657.511/(3.9241 - 0.44393 \cdot lg(P/1atm))$ and

$Ra_{cr} \approx 159.33 + 8.2324 \cdot P/1atm$ at the near-normal pressure $P \approx 1atm$.

The convective processes intensiveness can be influenced. The critical Rayleigh number $\mathrm{Ra}_{\mathrm{cr}}$ is weakly depending on the pressure, the intensiveness decreases as the pressure grows, changing from the maximum values at low pressure to minimal values at high pressure. Another and cardinal way to affect the intensiveness is to change the temperature. The intensiveness of convective processes is equal to zero at high and low temperatures and is different in between. Of course, it is possible to change both the pressure and the temperature.

In order to study the possibility to control convective processes by changing the pressure and the temperature in more details, consider the instability domain on *R-T* plane in Fig. 9.

A curve 1 in Fig. 9 correspond to the temperatures at which the maximum convection intensiveness at given pressure is observed (maximum C with respect to T corresponds to curve Ra_{cr}). Curves 2 and curve 3 correspond to the top and low boundaries of domain where reacting-inert gas transitions are observed.

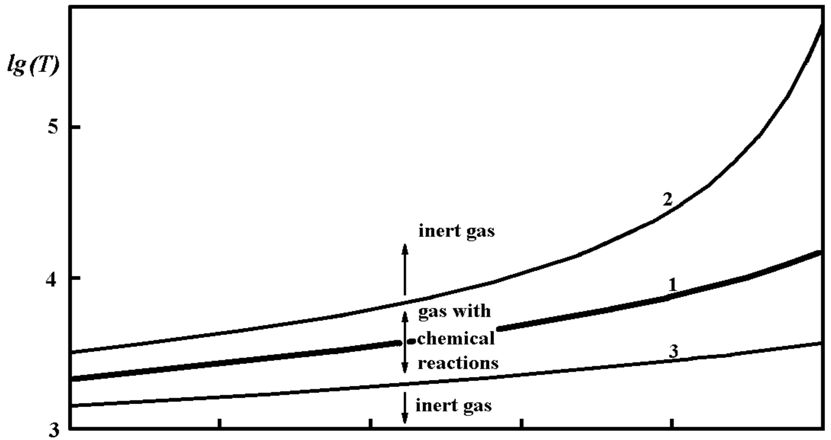

Fig. 9. The instability domain on the plane *R-T*

It is obvious that the highest increase in temperature by 155 times occurs at the upper boundary of the reacting-inert gas transition (curve 2), whereas the other curves demonstrate a substantially smaller change of temperature. For instance, at the lower boundary of the reacting-inert gas transition (curve 3), the change is by one order of magnitude less.

Curve 1 (the maximum convection intensiveness at given pressure) on the plane *R-T* is accurately described throughout the range of pressure change by

$$T(P) = \frac{1212.4}{1.2957 \cdot (P/1atm)^{-0.015848} - 1},$$

and at the near-normal pressure $P \approx 1atm$ by

$$T(P) = 3814.9 + 284.67 \cdot lg(P/1atm).$$

Similar approximate expressions for curves 2 and 3 on the plane *R-T*, where the top and low boundaries of the reacting-inert gas transition are realized as follow:

$$T(P) = 10^{\frac{3.8932 - 0.49630 \cdot \lg(P/1atm)}{1 - 0.15697 \cdot \lg(P/1atm) + 0.0013110 \cdot (\lg(P/1atm))^2}}$$ - for top curve 2

and

$$T(P) = \frac{2373.9}{1.4891 \cdot (P/1atm)^{-0.026968} - 1}$$ - for low boundary curve 3.

Considering the expressions above for $P \sim 1atm$, we obtain that:

$T(P) = 6922.0 + 897.84 \cdot P/1atm$ for curve 2 and

$T(P) = 1968.8 + 79.253 \cdot P/1atm$ for curve 3.

At the same time, the value of local maximum *C* that characterize the convection intensiveness vanishes in a practically linear way with respect to $lg(P)$:

$C(P) = 3.9241 - 0.44393 \cdot lg(P/1atm)$ along curve 1 and

$C(P) = 4.1169 - 0.19280 \cdot P/1atm$ at the near-normal pressure $P \approx 1atm$.

Conclusion

A new physical and mathematical model for convective flows of a gas in chemical equilibrium has been suggested. The flow is considered in a horizontal layer with heating from below. The gas is assumed to be viscous and incompressible, and the convective flow two dimensional and non-stationary. The horizontal boundaries of the layer are isothermal and free from shearing stresses. The parameters of the gas in chemical equilibrium (hydrogen-oxygen mixture) are calculated according to the model of chemical equilibrium proposed earlier. Given recombination and dissociation processes, an additional factor $C = C(T)$ appears as factor with the Rayleigh number in the system of equations describing convection. Hence, all the regimes and characteristics of convective flows of a chemical equilibrium gas can be derived from the corresponding characteristics of convection in a chemically inert medium when the Rayleigh number is overdetermined.

The results of linear analysis of the stability of a convective flow are presented. In particular, for a chemically active gas in equilibrium we obtained formula for the infinitesimal perturbation growth rate increments and formula for the critical Rayleigh number depending on temperature at given pressure. The neutral curve on the plane *T-Ra* shows the significant decreasing of the critical Rayleigh number in the reacting gas. The critical Rayleigh number (minimum with respect to *T*) depends on the pressure relatively weakly. The domain of the intensity convection increase due to chemical reactions in reacting gas on the plane *R-T* extends significantly towards higher temperatures when the pressure increases, which is especially true for the top high-temperature inert-reacting gas boundary.

Discussion

If we take into account recombination and dissociation processes, there appears an additional factor $C = C(T)$ with the Rayleigh number in the system of equations describing convection. Hence, all the regimes and characteristics of convective flows of a chemical equilibrium gas can be derived from the corresponding characteristics of convection in a chemically inert medium when the Rayleigh number is re-determined. In this respect, calculations of non-linear regimes of convection of a chemically active equilibrium gas yield little information.

In the present work the far-field high-temperature asymptotics for factor *C,* critical Rayleigh number and the increment λ is derived. It would be of certain interest to investigate also the low-temperature asymptotics.

The performed linear analysis shows the existence of the anomalous (non-monotonic) behavior of the thermal expansion coefficient in spite of the monotonic dependence of density on temperature. It seems to be possible that such anomalous (non-monotonic) behavior of the thermal expansion coefficient must bring to the secondary instability because of thermal expansion coefficient temperature dependence.

It would be of certain interest to prove experimentally the existence of the secondary instability because of thermal expansion coefficient temperature dependence. Another point of interest is related to the generation of the new physical and mathematical model and numerical investigation of such secondary instability. Of cause, the numerical investigation of this secondary instability must be performed with investigation of all regimes of flow together with defining the boundaries of temperature intervals where such regimes are observed, followed by researching integral characteristics, etc.

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