Rayleigh–Benard convection in a gas-vapor medium at the temperature close to the critical temperature

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Abstract. In this paper, we propose a new physico-mathematical model for the Rayleigh–Benard convection in a gas-vapor mixture of oxygen and cyclohexane, for which the temperature dependence of density has a maximum. Linear stability analysis was performed; two limiting cases where the inversion parameter tends to its limiting values are studied analytically. Formulas are obtained for the growth increment and decay, the neutral curve, and the boundary of the instability region in the wave plane.

1. Introduction

Convection in a medium with a monotonic temperature dependence of density has been well studied and described in numerous papers and books [1-3]. However, in nature and in a large number of important practical applications, e.g., in the convection of cold water during melting of glaciers [4-7], inert and reactive gas-vapor mixtures in chemical reactors, process plants, etc., the density of a convective medium is a non-monotonic non-linear function of temperature with a clear maximum at its certain (critical) value. The importance of the study of convection in such media is due to its numerous practical applications. The most complex problem of great theoretical and practical interest is to study the variety of convection modes in the vicinity of the maximum density point, where the buoyancy force changes sign when passing through zero [8].

The convection of a chemically inert gas-vapor mixture with a non-monotonic temperature dependence of density has been studied previously [9]. Gaseous oxygen with added liquid cyclohexane (the main raw material for the production of nylon, caprolactam, etc.) was considered as an inert medium, taking into account its evaporation and condensation at the boundaries of the volume. It has been shown that at a certain (critical) temperature, when all the added liquid cyclohexane evaporates, the density of the gas-vapor medium has a local maximum and the corresponding thermal expansion coefficient and the multiplier at the buoyancy term in the equations of motion changes sign when passing through zero.

Note that, in principle, such a gas-vapor mixture of oxygen and cyclohexane can undergo chemical transformations (the mixture is potentially explosive) if the fuel concentration is between the upper and lower concentration flammability limits. However, in this paper, as in [9], it is assumed that the fuel concentration is always outside the concentration flammability limits and the convective gas-vapor mixture is considered chemically inert.
We emphasize that the physically reasonable assumption of cyclohexane condensation on the solid walls of the volume and, hence, the formation of a more viscous liquid substance on the film walls allows the boundaries of the region to be considered as non-deformable and free of shear stress [10]. Analysis of the temperature dependence of the thermal expansion coefficient shows that it is advisable, as in [9], to assume that the thermal expansion coefficient is a piecewise constant function of temperature.

Note that the problem of Rayleigh–Benard convection in such a gas-vapor mixture asymptotically goes over into the classical Rayleigh problem of the convection of an incompressible fluid in a region with non-deformable horizontal boundaries free of shear stress if maximum density is reached at one of the horizontal boundaries [2].

We also note the obvious qualitative analogy with the penetrative convection of cold water at a temperature near the density maximum, where the thermal expansion coefficient, while being a linear function of temperature, also passes through zero [4]. This provides extensive theoretical and experimental data for comparison and verification of the proposed model [5 -7].

In particular, the analogy with the penetrative convection of cold water suggests that if the critical temperature is higher than the temperature of the cold boundary and lower than the temperature of the heated boundary, the maximum density line divides the whole layer into two sublayers, where instability can develop only in the lower sublayer, and the upper one is always stable. Moreover, the situation does not change qualitatively if the heating from below is replaced by heating from above [8].

As in cold water convection, decreasing the relative thickness of the lower unstable sublayer should lead to flow stabilization [4].

The objective of this paper are describe a new physico-mathematical model for the Rayleigh–Benard convection of a gas-vapor mixture of gaseous oxygen and cyclohexane vapor with the evaporation and condensation of cyclohexane and present the results of linear stability analysis and numerical calculations of nonlinear modes.

2. Physical properties of the gas-vapor medium

The convection of a gas-vapor mixture of gaseous oxygen $O_2$ and cyclohexane vapor $C_6H_{12}$ is considered taking into account the possible condensation of the latter at the boundaries of the region. For definiteness, the total mass fraction of cyclohexane (in the form of a condensed phase and vapor) is assumed to be $β_0 = 0.524$.

At the critical temperature $T_{cr}$, all the cyclohexane added to the system evaporates. Thus, at $T < T_{cr}$, cyclohexane is present in the system in the form of a liquid condensed phase at the boundaries of the region and in the form of saturated vapor, and increasing the temperature increases the saturated vapor pressure of cyclohexane (Fig. 1) and the density of the gas-vapor medium (Fig. 2). At $T > T_{cr}$, cyclohexane is present in the system only in the form of unsaturated vapor and its partial pressure changes relatively slightly, and further increase in temperature leads to a decrease in density in accordance with the ideal gas equation of state (Fig. 2).

It is assumed that all the boundaries of the region are impermeable. Using the Boussinesq approximation, in view of the small temperature change, the partial pressure of oxygen is assumed to be fixed and equal to $1 \text{ atm}$. The total pressure of the gas-vapor medium considered $P$ is equal to the sum of the partial pressures of oxygen and vapor $P = I + P_{sv}$.

At $T < T_{cr}$, the vapor pressure ($\text{atm}$) of cyclohexane can be calculated from the known absolute temperature [11]:

$$P_{sv}(T) = 9.87 \cdot 10^{2.9764 - \frac{1206.5}{T - 273.15 + 223.14}}.$$  \hspace{1cm} (1)

At $T > T_{cr}$, cyclohexane is present in the system only in the form of unsaturated vapor with a linear dependence of pressure on temperature in accordance with the ideal gas equation of state. Since, at $T > T_{cr}$, the rate of change of $P_{sv}$ with temperature is much lower than that at $T < T_{cr}$, the temperature dependence of $P_{sv}$ at $T > T_{cr}$ can be neglected (Fig.1).
The density of an ideal gas can be expressed as (Fig. 2):

\[
\rho(T) = \begin{cases} 
\frac{(1 + P_{sv}(T) \cdot \mu(T))}{RT}, & T \leq T_{cr} \\
\frac{(1 + P_{sv}(T_{cr}) \cdot \mu(T_{cr}))}{RT}, & T > T_{cr}
\end{cases}
\]

where \( P_{sv}(T_{cr}) \) and \( \mu(T_{cr}) \) are the saturated vapor pressure of cyclohexane and the molar mass of the gas mixture at \( T = T_{cr} \) and \( R \) is the universal gas constant. The temperatures of the cold and heated boundaries in Fig. 2 are shown conditionally to explain the problem statement and do not correspond to the real values.

In the density equation, the molar mass \( \mu \) is given by the formula (Fig. 3):

\[
\mu(T) = \frac{1}{1 + P_{sv}(T)} \left( \mu_{ox} + P_{sv}(T) \cdot \mu_{cy} \right) = \frac{1}{1 + P_{sv}(T)} \left( \frac{\mu_{ox} + P_{sv}(T) \cdot \mu_{cy}}{1 + P_{sv}(T)} \right) = \frac{1}{1 + P_{sv}(T)} \left( 3.2 + P_{sv}(T) \cdot 84 \right).
\]

Here \( \mu_{ox} = 32 \) and \( \mu_{cy} = 84 \) are the molar masses of oxygen \( \text{O}_2 \) and cyclohexane \( \text{C}_6\text{H}_{12} \), respectively. At \( T > T_{cr} \), the molar mass of the gas-vapor mixture is constant.

The thermal expansion coefficient \( \beta \) can be calculated from the following relation (Fig. 4):

\[
\rho = \frac{(1 + P_{sv}) \mu}{RT}, \quad \mu = \frac{1}{1 + P_{sv}} \left( 3.2 + P_{sv} \cdot 84 \right), \quad \beta = \frac{1}{\rho \frac{dT}{dT}} = \frac{1}{B \frac{dT}{dT}}, \quad B = (1 + P_{sv})(8 + 21 \cdot P_{sv})/T.
\]

The data in Fig. 4 show that the choice of the piecewise constant approximation of the temperature dependence of the thermal expansion coefficient is justified.
Thus, the thermal expansion coefficient is calculated as

$$\beta(T) = \begin{cases} -a = \beta(T_{cr} - 0) = -0.01583 & T \leq T_{cr}, \\ b = 1/T_{cr} = 0.003054 & T > T_{cr}. \end{cases}$$

In this connection, we note that in the vicinity of the critical temperature, the kinematic viscosity and temperature conductivity behave as continuous functions and, in the Boussinesq approximation, they can be considered constant.

The critical (maximum) saturated vapor pressure of cyclohexane can be expressed as a function of its total mass fraction (in the form of a condensed phase and vapor) $\beta_0$ and the corresponding value of the critical temperature is found by inverting the above relation (1). Thus, the accepted value $\beta_0 = 0.524$ corresponds to the critical values of the saturated vapor pressure $P_{sv} = 0.4191$ atm and temperature $T_{cr} = 54.32^\circ C$ (327.5 K).

It was noted above that the temperature of the cold upper horizontal boundary $T_c$ is lower than the critical value $T_{cr}$, and the temperature of the heated lower horizontal boundary $T_h$ is higher, and, hence, $T_c < T_{cr} < T_h$. As in the case of cold water convection, the maximum density line (where $T = T_{cr}$) divides the whole layer into two sublayers, where instability can develop only in the lower sublayer, and the upper sublayer is always stable [8]. The relative thicknesses of these sublayers are characterized by the inversion parameter $\tau = d/H = (T_h - T_{cr})/(T_h - T_c)$, $0 < \tau < 1$, which is the ratio of the height of the unstable sublayer $d$ to the thickness of the whole layer $H$. For $\tau = 1$, the above problem statement corresponds to the classical Rayleigh problem with $\beta = 0.003054$, and for $\tau = 0$ with $\beta = -0.01583$. As in the case of cold water convection, analysis of the density profile shape (see Figs. 2 and 5) shows that the situation does not change qualitatively if heating from below is replaced by heating from above [8].

3. Mathematical model

Arguing by analogy with [2], it can be obtained that, in the Boussinesq approximation, convection in the gas-vapor medium under consideration can be described by the following system of equations:

$$u_x + v_y = 0,$$

$$u_t + \frac{1}{Pr} (u u_x + v u_y) + P_x = \Delta u, \quad (2)$$

$$v_t + \frac{1}{Pr} (u v_x + v v_y) + P_y = \Delta v + \beta(T_{cr} + (Q + \tau - 1) \cdot \delta T) \cdot T_{cr} \cdot Ra \cdot Q,$$

$$Q_t + \frac{1}{Pr} (u Q_x + v Q_y) = \frac{1}{Pr} \Delta Q,$$

$$\beta(T_{cr} + (Q + \tau - 1) \cdot \delta T) \cdot T_{cr} = C(Q + \tau - 1), \quad C(Q + \tau - 1) = \begin{cases} 1, & Q \geq 1 - \tau, \\ -a/b = -5.183, & Q < 1 - \tau. \end{cases}$$

Here $u$ and $v$ are the velocities in the $x$ and $y$ directions, respectively, $Af = f_{xx} + f_{yy}$ is the Laplace operator, $v$ and $\chi$ are the kinematic viscosity and thermal diffusivity, and $\beta$ is the thermal expansion coefficient, which here is considered here as a function of the temperature $Q$. The kinematic viscosity and thermal diffusivity are considered constant. Here $Ra = g H^3 \delta T / (\chi v T_{cr})$ and $Pr = v/\chi$ are the Rayleigh and Prandtl numbers. The characteristic values of dimensional quantities are selected as follows: $H$ (height of the layer) for the length, $\chi/H$ for the velocity, $H^2/v$ for the time, $P_{0} \chi H^2$ for the pressure, $1/T_{cr}$ (the value in the unstable sublayer) for the thermal expansion coefficient, and $\delta T = T_h - T_c$ for the temperature; the inversion parameter $\tau = d/H = (T_h - T_{cr})/(T_h - T_c)$, $0 < \tau < 1$ is the ratio of the height of the unstable sublayer $d$ to the height of the whole layer $H$.

Figure 5 shows the initial linear profile and the boundary conditions for the temperature $Q = T - T_c$ and the velocity and the initial density profile.
Due to condensation and the formation of a film of liquid cyclohexane (which has a substantially higher viscosity than the convective gas-vapor mixture) at the boundaries of the region, all the boundaries of the region can be considered free of shear stress [7, 10].

The system of equations (2) was used in the numerical simulation of nonlinear Rayleigh-Benard convection modes.

![Diagram](image)

**Figure 5.** Boundary conditions for the velocity and temperature.

4. **Linear analysis**

Consider a linear analogue of system (2). Linearizing this system, introducing the stream function $\psi$ and vorticity $\omega$ according to formulas $u = \psi_y$, $v = -\psi_x$, and $\omega = v_x - u_y$ and replacing the temperature $Q$ by its deviation from the linear equilibrium distribution, we obtain the following system of equations:

$$
\omega_t = \Delta \omega + C(\tau, y) \cdot Ra \cdot Q_x, \quad \Delta \varphi = -\omega, \quad Q_t = (\Delta Q - \varphi_x) / Pr.
$$

(3)

Here the factor $C(\tau, y)$ is defined as

$$
C(\tau, y) = \begin{cases} 
1, & 0 \leq y \leq \tau, \\
-\alpha / b = -5.183, & \tau < y < 1.
\end{cases}
$$

Further, for simplicity, we redefine the parameter value $a = 0.01583$ by relating it to the value $b = 0.003054$ and assuming that $a = 5.183$. System (3) is solved in the region $G = \{(x, y)| 0 \leq x \leq L, 0 \leq y \leq 1\}$ with the boundary conditions equivalent to those shown in Fig. 5: $\psi = \omega = Q = 0$ for $y = 0, 1; 0 \leq x \leq L$ (on the horizontal boundaries) and $\psi = \omega = Q_x = 0$ for $x = 0, L; 0 \leq y \leq 1$ (on the vertical boundaries). Here $L$ is the dimensionless horizontal length of the region and $L = \pi$ in all calculations.

Stability of the equilibrium convection mode with respect to infinitely small perturbations is studied using the Galerkin method (finite $\tau$) [2; 12] and the orthogonalization method (infinitesimal low $\tau$).

In accordance with the Galerkin method, the approximate solution of system (3) is considered in the form

$$
\omega(t, x, y) = \exp(-\lambda t) \sin(\alpha x) \sum_{n=1}^{N} \omega_n \sin(n\pi y), \quad \psi(t, x, y) = \exp(-\lambda t) \sin(\alpha x) \sum_{n=1}^{N} \frac{\omega_n}{S_n} \sin(n\pi y),
$$

$$
Q(t, x, y) = \exp(-\lambda t) \cos(\alpha x) \sum_{n=1}^{N} Q_n \sin(n\pi y), \quad S_n = \alpha^2 + m^2 \pi^2.
$$

Here $\lambda$ is the eigenvalue (increment) and $\alpha$ is the wavenumber. Taking into account that

$$
\int_0^1 \sin^2(k\pi y) dy = \frac{1}{2}, \quad \int_0^1 \sin(n\pi y) \sin(k\pi y) dy = 0 \quad (m \neq k),
$$

and using the standard Galerkin procedure [12], we find that
\[-\lambda \omega_m = -S_m \omega_m + 2Ra \cdot \alpha \sum_{k=1}^{N} Q_k A_{mk}, \quad \lambda \Pr Q_m = S_m Q_m - \frac{\alpha}{S_m} \omega_m. \tag{4}\]

Here \( S_m = \alpha^2 + m^2 \pi^2, \quad 1 \leq k, m \leq N, \)

\[
A_{mk} = A_{km} = \frac{1}{2} \int C(r, y) \sin(m \pi y) \sin(k \pi y) dy, \quad A_{mk} = -(a+1) \left( \frac{\sin(2m \pi r)}{2m \pi} \right) / 2 - a / 2, m = k, \]

\[
A_{mk} = \frac{a+1}{\pi(k^2 - m^2)} (m \cos(m \pi r) \sin(k \pi r) - k \cos(k \pi r) \sin(m \pi r)), \quad m \neq k. \tag{5}\]

The condition for the existence of a nontrivial solution of system (4) can be written as

\[
\det(A - D) = 0, \tag{6}\]

where \( A \) is a square matrix with components \( A_{km} \) and \( D \) is a diagonal matrix with elements \( d_{mm} \):

\[
d_{mm} = \frac{S_m (S_m - \lambda)(S_m - \lambda \Pr)}{2Ra \cdot \alpha^2}, \quad 1 \leq m \leq N. \]

In the case of the neutral curve (\( \lambda = 0 \)), the relation for the diagonal matrix \( D \) is simplified to

\[
d_{mm} = \frac{S_m^3}{2Ra \cdot \alpha^2}, \quad 1 \leq m \leq N. \]

The obvious condition for the computational solvability of the unstable sublayer leads to a restriction on the minimum number of harmonics in the Galerkin method: the number of harmonics \( N \) must be greater than \( \tau^4 \) or \( N > \tau^4 \). The last relation indicates an unbounded increase in the number of harmonics increases in the calculations using the Galerkin method in the region of small values of \( \tau \). For small \( \tau \), the orthogonalization method is more effective.

Using the Maple 15 software for the calculations, from formula (6) we obtained a characteristic polynomial of degree \( 2N \) with respect to \( \lambda \), calculated the roots of this polynomial, and determined the neutral curve. In these numerical-analytical calculations, up to fourteen \( (N = 1, 2, \ldots, 14) \) harmonics were taken into account.

Consider now the asymptotic relations for \( \tau \to 1 \) when the density maximum is reached at the upper horizontal boundary and the problem in question is asymptotically transformed into the classical Rayleigh problem of convection in a region with non-deformable horizontal boundaries free of shear stress [2].

For \( A_{mk} \), we obtain

\[
A_{mk} = \frac{1}{2} \frac{1}{3} m^2 \pi^2 (1+a)(1-\tau)^3, \quad m = k, \quad A_{mk} = \frac{1}{3} mk \pi^2 (1+a)(1-\tau)^3 (1-\tau^4), \quad m \neq k. \]

The last relation shows that for as \( \tau \to 1 \), the equations for higher harmonics can be isolated and considered separately. However, it is these harmonics that determine the stability and characteristics of the flow [2, 3]. Moreover, test calculations have shown that, for \( \tau \to 1 \), the neutral curve and the perturbation growth increments can be calculated quite accurately using only one harmonic \( (N = 1) \).

For \( N = 1 \), the neutral curve takes the form

\[
Ra = \frac{S^3}{2A_1 \alpha^2}, \quad Ra = \frac{S^3}{\alpha^2} (1 + \frac{2}{3} \pi^2 (1+a)(1-\tau)^3) = \frac{S^3}{\alpha^2} (1 + 40.68 \cdot (1-\tau)^3), \quad S = \alpha^2 + \pi^2. \tag{7}\]

From this we find the critical value of the Rayleigh number (minimum of \( Ra \) as a function of \( \alpha \)):

\[
Ra = \frac{S^3}{2A_1 \alpha^2}, \quad Ra = \frac{S^3}{\alpha^2} (1 + \frac{2}{3} \pi^2 (1+a)(1-\tau)^3) = \frac{S^3}{\alpha^2} (1 + 40.68 \cdot (1-\tau)^3), \quad S = \alpha^2 + \pi^2. \tag{7}\]
It follows from relation (8) that

\[ Ra_{cr} = 6.75 \cdot \frac{\pi^4}{2A_1^4} = \frac{657.511}{2A_1} = 657.511 \cdot (1 + \frac{2}{3} \pi^2(1 + a)(1 - \tau)^3), \]

\[ Ra_{cr} = 657.511 \cdot (1 + 40.68(1 - \tau)^3), \quad \alpha_{cr} = 2.221. \]  

(8)

It follows from relation (8) that

\[ Ra_{cr} = 657.511 + O(1 - \tau)^3, \]

where the factor 657.511 is the critical Rayleigh number for the classical Rayleigh problem [2].

Relations (8) describe the asymptotics of the critical Rayleigh number and the corresponding critical wavenumber for \( \tau \to 1 \).

The critical Rayleigh number and the corresponding critical wavenumber are shown in Figs. 6 and 7. The solid curve shows the solution obtained using the orthogonalization method; the numbers at the dotted curves obtained by the Galerkin method correspond to the number of harmonics \( N \) considered in the calculations; the curve denoted as s1 corresponds to relation (8). The marks on the horizontal axis show the approximate limits of applicability corresponding to the selected number \( N \).

The similarity of the two curves (1 and s1) in Fig. 6 for \( 0.8 \leq \tau \leq 1 \) and their complete coincidence in Fig. 7 show that, for \( \tau \to 1 \), the calculated critical value of the Rayleigh number and the corresponding critical wavenumber have the theoretically established asymptotics. The position of the limit of applicability of the \( N \)-mode approximation is approximately inversely proportional to the number of harmonics taken into account, \( \tau = 1/N \). The data in Figs. 6 and 7 show that the single-mode approximation with \( N = 1 \) gives correct results for \( 0.8 \leq \tau \leq 1 \).

For the increment, we obtain

\[ \lambda = \frac{S}{2} \left( \frac{1 + Pr}{Pr} \right) - \sqrt{\frac{S^2}{4} \left( \frac{1 - Pr}{Pr} \right)^2 + \frac{2Ra \alpha^2 A_1}{SpR}}, \]

\[ \lambda = \frac{S}{2} \left( \frac{1 + Pr}{Pr} \right) - \sqrt{D + \frac{\pi^2(a + 1)Ra \alpha^2}{3PrS} \cdot (1 - \tau)^3}, \]  

(9)

\[ D = \frac{S^2}{4} \left( \frac{1 - Pr}{Pr} \right)^2 + \frac{Ra \alpha^2}{SpR}. \]

For \( Pr = 1 \), the expression for the increment is significantly simplified:

\[ \lambda = S - \alpha \sqrt{Ra/S} + \frac{\alpha \pi^2(a + 1) \sqrt{Ra/S} \cdot (1 - \tau)^3}{3}, \]

\[ \lambda = S - \alpha \sqrt{Ra/S} + 20.34 \cdot \alpha \sqrt{Ra/S} \cdot (1 - \tau)^3. \]  

(10)

It follows from relations (9) and (10) that the obtained values of the increment \( \lambda \) differ by an order of magnitude \( O(1-\tau)^3 \) from the corresponding value obtained for the classical Rayleigh problem and that decreasing the value of \( \tau \) leads to stabilization of the flow.

The growth increment \( \lambda \) as a function of the wavenumber is given in Fig. 8, where the numbers at the curves are the corresponding values of \( \tau, Ra = 10 Ra_{cr}, Ra_{cr} = 657.511 \), and \( Pr = 0.71 \).
It follows from relations (9) and (10) for the increment $\lambda$ and from the data in Fig. 8 that the value of the additional term increases according to the square root law as a function of the Rayleigh number and linearly as a function of the wavenumber $\alpha$ for $\alpha \ll \pi$.

For $\alpha \gg \pi$, the value of the additional term tends to the asymptotic value

$$\frac{\pi^2(a+1)}{3} Ra \cdot (1-\tau)^3 = 20.34 Ra \cdot (1-\tau)^3.$$

Figure 9 shows the region of instability in the wave plane, where $\alpha$ and $m$ are considered continuous and positive. The solid curve shows the boundary of the instability region for the Rayleigh problem ($\tau = 1$), and the dashed curves show the boundaries for $\tau = 0.8$ and 0.85. One can see that the instability region in the wave plane (flow stabilization) gradually decreases with decreasing $\tau$.

The curves in polar coordinates in Fig. 9 correspond to the equations

$$\alpha / Ra^{0.25} = \rho_v \cos(\varphi), \quad m \pi / Ra^{0.25} = \rho_v \sin(\varphi),$$

$$\rho_v = \cos^{0.5}(\varphi) \cdot (1 + a)(1 - \tau)^3 = \cos^{0.5}(\varphi) \cdot (1 - 10.17 \cdot (1 - \tau)^3),$$

$$0 \leq \varphi \leq \pi / 2.$$

Examining the asymptotics for $\rho_v(\varphi)$ as $\varphi \to 0$ ($m\pi \to 0$) and $\varphi \to \pi/2$ ($\alpha \to 0$), we obtain

$$\rho_v(\varphi) = 1 - \frac{\pi^2}{6}(1 + a)(1 - \tau)^3 = 1 - 10.17 \cdot (1 - \tau)^3.$$
In Fig. 9, the asymptotics $\rho_{w1}$ and $\rho_{w2}$ are shown by the dash-doted curves denoted by figures 1 and 2, respectively. It can be seen that, regardless of the chosen value of $\tau$, the asymptotics intersect at $\phi = 1.034$ at the point (0.375, 0.630). We can write the following relations based on the asymptotic expansions for the boundary of the instability region:

$$\alpha = B Ra^{0.25} (1 - \varphi^2 / 4) \cdot \cos(\varphi), \quad m \pi = B Ra^{0.25} (1 - \varphi^2 / 4) \cdot \sin(\varphi), \quad at \quad 0 \leq \varphi \leq 1.034,$$

$$\alpha = B Ra^{0.25} (\pi / 2 - \varphi)^{0.5} \cdot \cos(\varphi), \quad m \pi = B Ra^{0.25} (\pi / 2 - \varphi)^{0.5} \cdot \sin(\varphi), \quad at \quad 1.034 < \varphi \leq \pi / 2,$$

$$B = 1 - \frac{\pi^2}{6} (1 + a)(1 - \tau)^3 = 1 - 10.17 \cdot (1 - \tau)^3.$$

Considering the above relations for $\varphi \to 0$ and $\varphi \to \pi/2$ and retaining the first terms of the expansions, we obtain the following asymptotics:

$$\frac{\alpha}{B Ra^{0.25}} = 1 - \frac{3}{4} \left( \frac{m \pi}{B Ra^{0.25}} \right)^2, \quad \varphi \to 0; \quad \frac{\alpha}{B Ra^{0.25}} = \left( \frac{m \pi}{B Ra^{0.25}} \right)^3, \quad \varphi \to \pi / 2.$$

Thus, asymptotically as $\varphi \to 0$ and $\varphi \to \pi/2$, the boundary of the instability region in the wave plane takes the form of a quadratic or cubic parabola, respectively, and, in these variables, it has a universal form, shown by the solid curve in Fig. 9.

We now consider the limiting relations for $\tau \to 0$.

For $A_{mk}$ we can write

$$A_{mk} = -\frac{1}{2} \alpha + \frac{1}{3} m^2 \pi^2 (1 + a) \tau^3, \quad m = k; \quad A_{mk} = \frac{1}{3} mk \pi^2 (1 + a) \tau^3, \quad m \neq k.$$

The latter relation shows that for $\tau \to 0$, the equations for the first harmonics can be isolated and considered separately. From the above expression for the neutral curve (7), it follows that all perturbations decay as $\tau \to 0$.

It can be shown that the decaying perturbations for $\tau \to 0$ have a typical oscillatory nature. In fact, there exists a wavenumber value for which two real branches of the single-mode solution merge to form a complex conjugate pair if the Rayleigh number exceeds the threshold value $(Pr = 0.71)$ is equal to 3.757 [2].

The obtained value is very small since it is 175 times smaller than the critical value for the classical Rayleigh problem.

We write the ratio for the increment for $\tau \to 0$, assuming for simplicity that $Pr = 1$ (in other words, assuming that the threshold value of the onset of oscillations is zero):

$$\lambda = S - i \alpha \sqrt{Ra / S} \cdot (1 - \frac{\pi^2 (1 + a)}{3a}) \cdot \tau^3, \quad \lambda = S - 2.277 i \alpha \sqrt{Ra / S} \cdot (1 - 3.925 \tau^3).$$

It can be seen from the above relation that the decay rate, determined by the real part of the increment, does not depend on the inversion parameter $\tau$, and its increase (decrease) leads to only a slight decrease (increase) in the oscillation frequency.

Compare now the critical Rayleigh numbers and their corresponding critical wavenumbers obtained in the present work, for convection in cold water [5–7], and in the classical Rayleigh problem with non-deformable free boundaries [2]. For the data in Figs.10 and 11 given below, the height of the unstable sublayer is taken as the length scale, and the values of the critical Rayleigh number and the wavenumber are recalculated as $Ra_{cr} \tau^4$ and $a_{cr} \tau$, respectively.

In Figs. 10 and 11, the solid curves show the results of this work (curve 1) and calculated data on convection in cold water [6] (curve 2), the points correspond to the calculated data on convection in cold water [5], and the dotted curve shows the result of solving the classical Rayleigh problem [2]. In Fig. 10, the dash-dotted curve shows the experimental data on convection of cold water poured on ice [7]. Compare now the critical Rayleigh numbers and their corresponding critical wavenumbers obtained in the present work, for convection in cold water [5–7], and in the classical Rayleigh problem with non-
deformable free boundaries [2]. For the data in Figs. 10 and 11 given below, the height of the unstable sublayer is taken as the length scale, and the values of the critical Rayleigh number and the wavenumber are recalculated as $\text{Ra}_{cr} \cdot \tau^4$ and $\alpha_{cr} \cdot \tau$, respectively.

In Figs. 10 and 11, the solid curves show the results of this work (curve 1) and calculated data on convection in cold water [6] (curve 2), the points correspond to the calculated data on convection in cold water [5], and the dotted curve shows the result of solving the classical Rayleigh problem [2]. In Fig. 10, the dash-dotted curve shows the experimental data on convection of cold water poured on ice [7].

It can be seen from the data in Figs. 10 and 11 that, for $0.8 < \tau \leq 1$, the results of the present work are close to the calculated data for convection in cold water [5, 6]; for $\tau = 1$, they coincide with the results of solving the classical Rayleigh problem; and in the region of small $\tau$, they asymptotically reach constant values.

From the data in Figs. 10 and 11, we can obtain the asymptotics the critical Rayleigh number $\text{Ra}_{cr} = 526.4/\tau^4$ and the corresponding critical wavenumber $\alpha_{cr} = 2.122/\tau$ as $\tau \to 0$. Note that the experimental data on the critical Rayleigh number for convection in cold water [7] are much closer to the results of the present work (deviation of 9.6%) than to the theoretical results for convection in cold water [5, 6], where the deviation was about 43%. This may be due to the fact in the experimental study [7], as in the present work, the thermal expansion coefficient $\beta$ was considered constant and equal to the arithmetic mean of its values at the horizontal boundaries. For the same reason, the results of the present work are also much closer to the results of solving the classical Rayleigh problem (with constant $\beta$) than are the theoretical results for convection in cold water [5, 6].

5. Numerical method

The system of equations (2) is replaced by its discrete analogue constructed using a staggered finite volume method. In the vertical direction, we use a non-uniform difference grid refined near the upper and lower horizontal boundaries. The scheme is fully implicit in time and central-difference in diffusion terms. The QUICK scheme is used for convective terms, and the SIMPLE algorithm for pressure calculations. The pressure is determined from the Poisson equation using the Bi-CGSTAB algorithm. The numerical algorithm gives a second-order approximation in space and time. A more detailed description of the numerical method can be found in [13].

In the calculation results presented here, the whole flow region $(x, y) = ([0, \pi], [0, 1])$ is discretized using $80 \times 40$ points for $\tau \geq 0.5$ and $120 \times 60$ points for $\tau < 0.5$. The sufficiency of the spatial resolution was verified by calculations for $\tau = 0.1$ on a grid of $300 \times 150$ cells. The dimensionless time step is chosen in the range from $10^{-8}$ to $10^{-5}$.

6. Numerical simulation results

The critical Rayleigh numbers obtained in this work using linear theory and by the numerical calculation using the nonlinear equations (2) show a agreement with graphical accuracy.

As noted above, if the critical temperature is between the temperatures of the upper and lower horizontal boundaries, the maximum density line divides the whole layer into two sublayers, where
instability can develop only in the lower layer, and the upper sublayer is always stable. The relative thickness of the unstable underlayer increases with increasing inversion parameter. As a result, the fluid layer generally becomes more unstable, and the critical Rayleigh number decreases.

Slightly supercritical stationary flow (here $Ra \approx Ra_{cr}(\tau)$) for different inversion parameters is shown in Fig. 12, where the plus sign corresponds to clockwise rotation and the minus sign to counter clockwise rotation.

The convective flow for $\tau = 1.0$ consists of a pair of vortices rotating in opposite directions. In this case, the flow occupies the whole layer, as is evident from Fig. 12 (a). As the inversion parameter decreases, the maximum density line gradually moves to the lower boundary and the relative thickness of the upper stable sublayer increases. Fluid flow of relatively low intensity in the upper, always stable, sublayer is due to the presence of rotating vortices in the lower sublayer and viscosity. As a result, the directions of rotation of the vortices in the upper and lower sublayers are opposite, as shown in Fig. 12 (c-d). With a further decrease in the inversion parameter, flow is almost completely suppressed in the upper sublayer and is observed only in the lower sublayer, as shown in Fig. 12 (e-f). It should be noted that the number of vortices increases with decreasing inversion parameter.

Figure 12. Isolines of the stream function for different inversion parameters.

Figure 13 shows the stationary solution for the temperature and stream function fields for different Rayleigh numbers and inversion parameters. When the Rayleigh number is slightly higher than the critical value (Fig. 13, and at $Ra = 710$), the flow is relatively weak and heat is mainly transferred by conduction. As a result, isotherms are seen as a set of horizontal parallel lines. With an increase in the Rayleigh number, the flow intensity increases and the upward flow between two cells causes an increasing deformation of the isotherms, as can be seen in Fig. 13, a for $Ra = 10^3$ and $10^5$. A comparative analysis of the data obtained by calculations for different inversion parameters (Fig. 13, a-c) shows that as the inversion parameter decreases, the upper stable fluid layer becomes thicker and, as a result, there is always a motionless fluid layer near its upper boundary where isotherms also appear as a set of horizontal parallel lines. However, the existence of Rayleigh–Benard convection in the lower unstable layer causes an increase in the temperature gradient near its upper boundary. It should be noted that the isotherm lines are strongly deformed in the lower unstable layer for a small inversion parameter, as shown in Fig. 13 (b) and (c).
Figure 13. Stationary convection mode for different values of $\tau$ and Rayleigh numbers. Isotherms are shown at the top, and stream function isolines at the bottom.
7. Discussion
As noted above, a gas-vapor mixture of oxygen and cyclohexane is explosive if the concentration of the fuel (cyclohexane) is between the upper and lower concentration flammability limits. In this paper, it is assumed that the fuel concentration is always outside the concentration flammability limit and the convective gas-vapor mixture is considered chemically inert. However, convective movement can change the fuel concentration, resulting in the formation of local regions where the fuel concentration is within the concentration flammability limits and the mixture becomes explosive. A natural question that arises here is: What are the conditions for the formation of local regions with the explosive mixture. Due to its great practical importance, this question should be carefully investigated.

Another interesting problem arises from the comparison of the wavenumbers in Fig. 11 (linear theory) and Fig. 13 (stationary solutions at low supercriticality) for small $\tau$. As noted above, the critical wavenumber based on linear theory increases inversely with the inversion parameter, but, at the nonlinear stage (Fig. 13), the number of observed vortices is several times smaller. This suggests that the nonlinear development of finite-amplitude perturbations leads to the formation of an effective value of the inversion parameter greater than the specified value. In other words, finite-amplitude perturbations increase the effective thickness of the unstable sublayer. However, increasing the inversion parameter automatically decreases the critical Rayleigh number. Thus, in this case, subcritical finite-amplitude convection should be observed, which is of both theoretical and practical interest.

Conclusion
In this paper, we described a new physico-mathematical model for convection of a gas-vapor mixture of gaseous oxygen and cyclohexane vapor, taking into account the evaporation and condensation of cyclohexane at the boundaries of the region. It is shown that at a certain (critical) temperature at which all the added liquid cyclohexane evaporates, the density of the gas-vapor medium reaches a local maximum at which the thermal expansion coefficient and the buoyancy force in the equations of motion change sign when passing through zero.

Linear stability analysis was carried out, and the results of numerical calculations of nonlinear stationary Rayleigh–Benard convection modes were analyzed.

The physically reasonable assumption of cyclohexane condensation on the solid walls of the volume and, hence, the formation of a more viscous liquid substance on the film walls made it possible to consider the boundaries of the region non-deformable and free of shear stress, which significantly simplified the consideration. In this case, it is advisable to consider the thermal expansion coefficient as a piecewise constant function of temperature.

The problem of Rayleigh–Benard convection in the gas-vapor mixture under consideration asymptotically passes to the classical Rayleigh problem of convection of an incompressible fluid in a region with non-deformable horizontal boundaries free of shear stress if maximum density is reached at one of the horizontal boundaries and, consequently, the inversion coefficient is 0 or 1. In both limiting cases, asymptotics for the critical Rayleigh number and the corresponding critical wavenumber were derived.

It is shown that there is a qualitative analogy between convection in the gas-vapor medium under consideration and penetrative convection of cold water near the maximum density point, where the thermal expansion coefficient also passes through zero, but is considered a linear function of temperature.

It is noted that if the critical temperature is higher than the temperature of the cold boundary and lower than the temperature of the heated boundary, then, as in convection of cold water, the density maximum line divides the whole layer into two sublayers, where instability can develop in the lower one, and the upper sublayer is always stable. Moreover, the shape of the density profile shows that the situation does not change qualitatively if heating from below is replaced by heating from above.

The solution of the linear stability problem shows that decreasing the relative thickness of the lower unstable sublayer or, in other words, increasing the relative thickness of the upper stable sublayer leads to flow stabilization.
Two asymptotic cases with $\tau \to 1$ and $\tau \to 0$ are analyzed using linear theory. It is shown that behavior of the solution is described by the equation for the first mode. In a single-mode approximation, expressions for the growth increment of the harmonic perturbation were obtained and the boundary of the instability region in the wave plane was investigated.

It is shown that when $\tau \approx 1$, decreasing the inversion parameter $\tau$ leads to an increase in the flow stability, and when $\tau \approx 0$, it leads to an increase in the frequency of decaying oscillations, while the decay rate remains unchanged.

Numerical calculations of nonlinear stationary convection modes were performed using a numerical finite volume method for different inversion parameters and Rayleigh numbers. The calculated values of the critical Rayleigh number are in good agreement with linear stability theory.

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