Numerical study of bulk condensation in laminar flow diffusion chamber

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Abstract. The process of bulk condensation was studied on a basis numerical solution of kinetic equation for the mass distribution function of droplet size and the equations of mass and energy balance. The effect of the condenser and preheater deference temperature was studied. Obtained results were compared with other authors’ experimental and numerical data qualitatively and quantitatively.

1. Introduction
The bulk condensation consists of two main processes: formation of a liquid droplets (nucleation) and growth condensed particles. Nucleation has been studied over 100 years, but this phenomenon is still poorly understand. Experimental homogenous nucleation studies have been usually done with an expansion cloud chamber and a static diffusion chamber. The nucleation rate range of these devices does not overlap. The nucleation rate range of the laminar flow diffusion chamber fills this gap between these two devices.

The laminar flow diffusion chamber (LFDC) consists of three main elements: saturator, preheater and condenser. The carrier gas is saturated with the vapor by evaporation liquid phase. The vapor – gas mixture moves into the preheater, where it is heated to prevent its condensation on the wall. In the condenser, the mixture is cooled by heat exchange with cold walls. Supersaturation is achieved because of saturation pressure of vapor is a strong exponential function of temperature. If this supersaturation is high enough, the process of bulk condensation begins.

The aim of this study is simulation of bulk condensation in the LFDC using methods of the continues matter mechanics and physical kinetics.

2. Formulation of the problem and mathematical description
We consider the stationary laminar flow of the vapor – gas mixture in the condenser of the LFDC. The inner diameter of tube is much larger than the mean free path, so the continues matter mechanics is used for the description of the flow, but not for the interaction of gaseous phase and droplets. The velocities of liquid and gaseous phases were assumed to be identical because the droplets size is small. The temperature of the droplets is equal to the temperature of the mixture, this approach is justified by the low concentration of vapor in comparison with gas [1]. The temperature of the saturator, preheater and condenser and the volumetric flow rate and total pressure of the mixture are given.
The velocity profile is approximated by the parabolic profile for laminar flow:

\[ u = \frac{2V}{\pi R_0^2} \left[ 1 - \left( \frac{y}{R_0} \right)^2 \right]. \]  

Here \( V \) is the volumetric flow rate of mixture, \( R_0 \) is inner radius of the tube and \( y \) is radial coordinate. The volumetric flow rate is assumed to be constant along the whole tube. This hydrodynamic model simplifies solution of the problem.

We used the equations of mass and energy balance to describe the distributions of temperature and relative density of vapor which are written as follows:

\[ u \frac{\partial C_v}{\partial x} = D \left[ \frac{1}{y} \frac{\partial C_v}{\partial y} + \frac{\partial^2 C_v}{\partial y^2} \right] - \frac{1}{\rho} l_v, \]

\[ u \frac{\partial T}{\partial x} = a \left[ \frac{1}{y} \frac{\partial T}{\partial y} + \frac{\partial^2 T}{\partial y^2} \right] + \frac{L}{\rho c_p} l_v, \]

where \( C_v \) is relative density of vapor, \( x \) is axial coordinate, \( T \) is the temperature, \( \rho \) the density of vapor – gas mixture, \( D \) is the diffusion coefficient, \( a \) is thermal diffusivity, \( c_p \) is the specific heat capacity at constant pressure and \( L \) is evaporation heat. The second term in the right parts of the equations (2) and (3) describe decrease of vapor’s mass and heat release due to bulk condensation.

The kinetic equation for droplet size distribution function is used for description of bulk condensation of supersaturated vapor. Taking into account parabolic velocity profile (1) and stationary flow this equation [2] is written as follows:

\[ u \frac{\partial f}{\partial x} + \frac{\partial (rf)}{\partial r} = \frac{J}{\rho} \delta (r - r_{cr}). \]

Here \( f \) is the mass distribution function of droplet size, \( r \) is the droplet radius, \( J \) is the nucleation rate, \( r \) is the droplet growth rate, \( \delta \) is the delta function and \( r_{cr} \) is the critical droplet radius. The aerosols parameters (number of droplets per volume unit, mass fraction of liquid phase) are defined as moments of the distribution function.

Integral term in the equations of mass and energy balance (2) and (3) was calculated using the follow formula:

\[ l_v = \frac{4}{3} \pi r_{cr}^3 \rho_{\text{liq}} J + \rho_{\text{liq}} 4\pi \int_{r_{cr}}^{\infty} r^2 (rf) \, dr, \]

where \( \rho_{\text{liq}} \) is the density of liquid phase. The first and the second terms describe decrease of vapor’s mass due to the formation of new aerosol particles and growth of droplets, respectively.

We use the well know Frenkel-Zeldovich formula [3] for calculating the nucleation rate in (4) and (5). The growth rate in (3) and (4) was calculated with the use of the Fuchs formula [4]:

\[ \dot{r} = \beta \frac{p_v - p_s(T)}{\rho_{\text{liq}}} \frac{1 + \beta \left[ \frac{RT}{2\pi R} \frac{r^2}{r + \langle l \rangle} \right]^{1/2}}{\sqrt{2\pi RT}}. \]

Here \( \beta \) is the condensation coefficient, \( p_v \) and \( p_s(T) \) are partial pressure of vapor and saturation pressure of vapor at the temperature of the mixture, \( R \) is the individual gas constant and \( \langle l \rangle \) is the mean free path.
One more equation should be added to the system of equations (1-6) to couple it. It was the perfect gas equation of state for gaseous phase.

The equations (1-6) are solved with the following boundary conditions:

\[ T(0, y) = T_{\text{preh}}, \]
\[ T(x, R_y) = T_{\text{cond}}, \tag{7} \]
\[ \frac{\partial T(x, 0)}{\partial y} = 0, \]
\[ C_v(0, y) = C_v(T_{\text{sat}}), \]
\[ C_v(x, R_y) = C_v(T_{\text{cond}}), \tag{8} \]
\[ \frac{\partial C_v(x, 0)}{\partial y} = 0, \]
\[ f(0, y, r) = 0. \tag{9} \]

The system of equations (1-6) with boundary conditions (7-9) is solved with the program developed by authors using finite difference method for the equations of mass and energy balance [5] and the method of direct numerical solution for the kinetic equation [6].

3. Result and discussion

The calculations were carried out for the mixture of n-butanol (vapor) and helium (gas). The temperature of saturator was 302 K, the temperature of preheater was 310 K and the temperature of condenser was variated from 280 K to 265 K. The volumetric flow rate of the mixture was 15 cm$^3$s$^{-1}$, the total pressure was 101325 Pa.

The profiles of droplets' number per volume unit at $y = 0$ are presented in figure 1. It can be seen that number of droplets increases with decrease of the temperature of condenser. The profile of mass fraction at $y = 0$ is shown in figure 2. The mass fraction of liquid is negligible at 280 K. There is maximum mass fraction of liquid at the temperature between 275 K and 270 K.

Decrease of the temperature of condenser (increase of the temperature difference between condenser and preheater) makes heat transfer with cold walls more intensive, so supersaturation ratio (partial pressure of vapor divided by its saturation pressure at temperature of the mixture) increases faster and its maximal value increases. Therefore, the bulk condensation becomes more intensive at higher temperature difference.

Number of droplets per volume unit and mass fraction of liquid on the chenal axis at $x = 8$ cm as functions of temperature difference between condenser and preheater $\Delta T$ are presented in figure 3 and figure 4. Number of droplets increases monotonically with increase of $\Delta T$. Mass fraction of liquid has more complex dependence on $\Delta T$ than numerical density of droplets. This fact is caused by that mass fraction of liquid phase increases due to nucleation and growth droplets, number of droplets increases due to nucleation only. The comparison of figure 3 and figure 4 shows that growth of droplets is the most intensive when the difference of temperature of the condenser and preheater is between 35 K and 40 K.
Figure 1. The profile of number of droplets per volume unit on the chenal axis at different values of $T_{\text{cond}}$

Figure 2. The profile of mass fraction of liquid on the chenal axis at different values of $T_{\text{cond}}$

Figure 3. Number of droplets per volume unit as a function of condenser and preheater difference temperature

Figure 4. Mass fraction of liquid phase as a function of condenser and preheater difference temperature

The profiles of the temperature (a), relative density of vapor (b) and supersaturation ratio (c) at $y = 0$ obtained with and without bulk condensation are shown in figure 5 (the temperature of the condenser is 265 K). It is easy to see that curves in figure 5(a) is very close. The heat release due to the bulk condensation is negligible. The relative density of vapor decreases strongly when the nucleation begins. Supersaturation ratio decreases due to formation of condensed particles and its growth. It should be noted that effect of the bulk condensation on the relative density of vapor and supersaturation is strong if condensation is intensive enough.
Figure 5. The profiles of temperature (a), relative density of vapor (b) and supersaturation ratio (c) on the chenal axis. Solid lines are results with account for bulk condensation and dash line are ones without it.

Comparison of obtained results with experimental and numerical data [7] is presented in figure 6. In general, qualitative and quantitative agreement with numerical results of [7] can be seen. However, comparison with the experimental data [7] gives only a qualitative agreement. It is due to the use of the Frenkel-Zeldovich formula for calculating the nucleation rate, which leads to of several orders difference with the experiments, depending on the partial pressure of vapor.

Figure 6. The axial profiles of temperature (a), supersaturation (b) and nucleation rate (c) on the chenal axis. Black and grey dots are other authors’ numerical and experimental data [7], respectively. Solid lines are our results.

4. Conclusion
The calculations showed that intensively of condensation depends on condenser and preheater difference temperature. The mass fraction of the liquid increases mainly due to the nucleation process at higher temperature differences, and at low temperatures drops the growth prevails. It was also found that there is a certain value of the temperature difference at which the growth of droplets is most intense.

The process of intense bulk condensation has a significant effect on the distribution of relative vapor density and supersaturation ratio. Due to the formation and subsequent growth of condensed particles, the relative density of the vapor and supersaturation ratio rapidly decrease.

When comparing the results obtained with the calculated data of other authors, qualitative and quantitative agreement was obtained, and comparison with the experimental data on the rate of nucleation gave only qualitative agreement.
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