PAMM · Proc. Appl. Math. Mech. **7**, 2100029–2100030 (2007) / **DOI** 10.1002/pamm.200700233

Non-equilibrium gas-liquid transition model

Bronislav V. Librovich [*], **Andrzej F. Nowakowski** [**2], **Issa Chaer** [3], and **Savvas Tassou** [3]

[2] Mechanical Engineering Department, Sheffield University, Sheffield S1 3JD, UK.
[3] School of Engineering and Design, Brunel University, Uxbridge, Middlesex UX8 3PH, UK.
[1] RAF Group, Pereulok Chernyshevskogo 15, Moscow, 127473, Russia.

A new rigorous mathematical model for evaporation/condensation, including boiling, has been proposed. A problem of phase transition and in particular evaporation/condensation is one of the most acute problems of modern technology with numerous applications in industry, such as: in refrigeration, distillation in chemical industry. It is very common to use equilibrium evaporation model, which assumes that concentrations of species in the gas phase is always at saturated condition. Such kind of approach can lead to significant errors, resulting in negative concentrations in complex computer simulations. In this work two analytical solution of simplified differential-algebraic system have been obtained. One of them was deduced using assumption that the process is isothermal and gas volume fraction is constant. In the second solution the assumption about gas volume fraction has been removed. The code for numerical solution of differential-algebraic system, using conservative scheme, has been developed. It was designed to solve both systems of equations with boiling and without. Numerical calculations of ammonia-water system with various initial conditions, which correspond to evaporation and/or condensation of both components, have been performed. It has been shown that, although system quickly evolves to quasi equilibrium state (the differences between current and equilibrium concentrations are small) it is necessary to use non-equilibrium evaporation model, to calculate accurately evaporation/condensation rates, and consequently all other dependent variables.

Introduction

A problem of phase transition, and in particular evaporation/condensation, is one of the most acute problems of modern technology. There are numerous applications of this process in industry, for example, in refrigeration, and chemical industry.

It is very common to use an equilibrium evaporation model, which assumes that concentrations of species in the gas phase is always at saturated condition [1, 2]. This approach is not only conceptionally questionable, indeed, if gas is at saturated condition there is no evaporation or condensation, but sometimes can lead to significant numerical errors, negative concentrations, etc. in complex computer simulations. Therefore, for some industrial problems, for example, modelling of absorption refrigeration cycle, it is absolutely necessary to develop and use non-equilibrium evaporation/condensation model [3, 4].

Mathematical model

The main assumptions for the model are:

- There is thermal equilibrium between two phases. Namely, temperature of gas is equal to liquid temperature, $T_g = T_l$.
- There is mechanical equilibrium between two phases, gas and liquid pressures are equal. The pressure gradient due to gravity is neglected.
- The gas phase is considered as an ideal gas.
- The liquid phase is assumed to be incompressible.

Numerical Results

The numerical results in the following sections are related to the behaviour of a two component ammonia/water system. This kind of binary system is chosen due to its importance within the refrigeration industry.

In the considered problems there are two characteristic times, namely: 1) characteristic time, which is related to evaporation/condensation, τ_{ev}, 2) characteristic time, which is related to heating up/cooling, τ_h. Typically, evaporation characteristic time is much smaller than heating evaporation time, $\tau_{ev} \ll \tau_h$.

It is possible to show that for a short period, ($t \sim \tau_{ev}$) the influence of wall temperature (external heat flux) is insignificant. Therefore, in all calculations in this subsection, one value of wall temperature has been used, $T_w = 270$ K. In Fig. 1 profiles

---

[*] Corresponding author: e-mail: b.librovich@raf.ru [1]

[**] e-mail: A.F.Nowakowski@sheffield.ac.uk

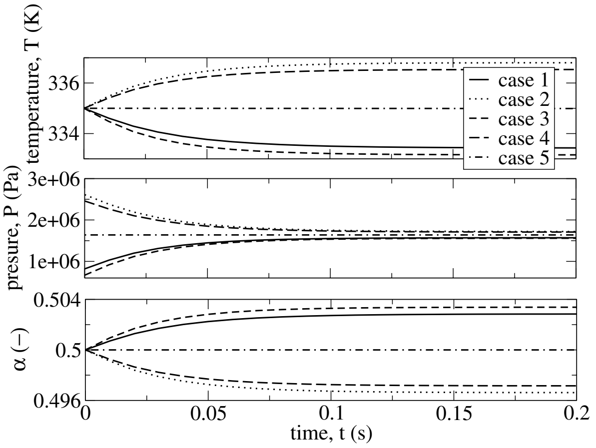

Fig. 1 The temperature, pressure and gas volume fraction profiles as function of time for the short period of calculation, $t \sim \tau_{ev}$.

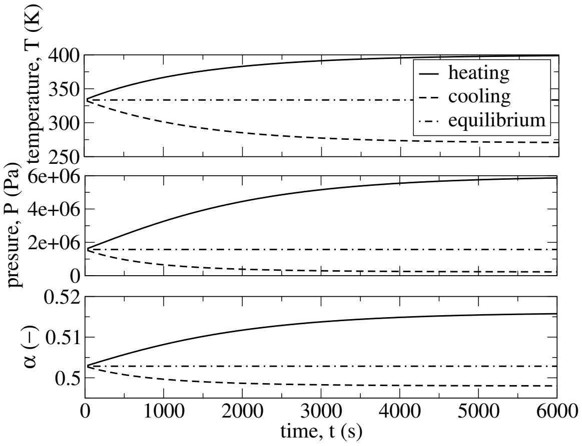

Fig. 2 The temperature, pressure and gas volume fraction profiles as function of time for the long period of calculation, $t \sim \tau_h$.

of temperature, pressure and gas volume fraction are presented for all five cases considered above. It is shown that all profiles display monotonic behaviour.

It is worth noting, that the pressures for all 5 cases do not approach one value. It happens due to the fact that for all 5 cases the initial conditions for gas concentrations are different, therefore, the total mass of the system is different for all cases. It causes the differences between concentration equilibrium pressures.

In the case of a long period of calculation ($t \sim \tau_h$) the initial conditions for gas concentrations are not so significant. For such long periods, external heat flux starts to play a significant role. Here, as opposed to the previous subsection, the initial conditions for gas concentrations are fixed and the wall temperature is varied in order to investigate the system dependence on external heat flux. Namely three cases are considered: 1) Heating, $T_w = 400$ K. In this case the external heat flux is positive, and the internal energy of the system is increasing in time. 2) Cooling, $T_w = 270$ K. The external flux is negative which causes a decrease in the internal energy. 3) Equilibrium, $T_w = 335$ K. In the thermal equilibrium external heat flux is zero and the system is in an equilibrium state. Initial conditions for gas concentrations for all cases in this subsection correspond to concentration equilibrium, $\tilde{C}^0_{g1} = \tilde{C}^{eq}_{g1}(\tilde{T}^0)$, $\tilde{C}^0_{g2} = \tilde{C}^{eq}_{g2}(\tilde{T}^0)$. In Fig. 2 the behaviour of temperature, pressure and gas volume profiles in time is presented for long period of calculations. The temperature of the system rises in time, in the case of heating external flux is positive. It approaches the wall temperature. The pressure also rises due to heating, and gas volume fraction increases due to evaporation. In the case of cooling, the external heat flux is negative. Therefore, in contrast to the previous case, temperature, pressure and gas volume fraction decrease during the process. In the thermal equilibrium case all dependent variables remain constant due to the fact that external heat flux is zero.

Conclusions

The main achievements of the current work are:

- A rigorous mathematical model of evaporation/condensation, including boiling, has been proposed.
- The code for the numerical solution of the differential-algebraic system has been developed. It was designed to solve both systems of equations with and without boiling and to switch from one regime to another, according to boiling condition.
- Numerical calculations of an ammonia-water system with different initial conditions, which correspond to evaporation and/or condensation of both components, and wall temperature have been performed.
- It has been shown that, although the system quickly evolves to quasi concentration equilibrium state (the difference between current and equilibrium concentrations are rather small) it is necessary to use the non-equilibrium evaporation model to calculate evaporation/condensation rates as well as all other dependent variables accurately.

References

[1] V. I. Makeyev, V. F. Pleshankov, A. P. Chuguev, Formation and burning of hydrogen-air mixtures in the process of evaporation of liquid hydrogen into the atmosphere, Fizika Goreniya i Vzryva, **5**, 14–21 (1981).

[2] N. I. Zverev, N. N. Smirnov, L. A. Dekhtyarenko, N. A. Shchepotyev, D. M. Yakubovich, Unsteady-state evaporation of liquid oxygen into the atmosphere., Fizika Goreniya i Vzryva, **2** (3), 73–78 (1989).

[3] R. G. Remorov, M. W. Bardwell, Langmuir approach in the study of interface mass transfer, Surface Science, **585**, 59–65 (2005).

[4] V. Chernyak, The kinetic theory of droplet evaporation, Journal of Aerosol Science, **26**(6), 873–885 (1995).