Thermodynamics of growth or evaporation of a multicomponent droplet

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Abstract

Detailed description of stationary and non-stationary thermodynamic characteristics of growing or evaporating multicomponent droplets is of great importance for general study of phase transitions, for understanding the aerosol processes in the Earth's atmosphere [1], for such technological applications as efficient combustion of dispersed liquid fuel [2] or producing nanoparticles with a controlled size, morphology, and composition in spray pyrolysis based on multicomponent droplet-to-particle conversion [3]. New intensively developing optical techniques for tracking the changes in temperature and chemical composition of small droplets in situ [4] extend the requirements to the modern theory of droplet condensation and evaporation.

Thermodynamics allows one to find the evaporation rates for a multicomponent droplet and relate them to the chemical composition, size and temperature of the droplet. The conditions of a preservation of the matter and enthalpy in the thermally isolated system (which includes the droplet and the vapor-gas shell around the droplet affected by the vapor component fluxes) lead to the material and enthalpy balance equations regulating the behavior of the droplet and vapor-gas environment. On a such thermodynamic basis, we present in this report a rigorous derivation of a new set of equations for the size, composition and temperature of a small multicomponent droplet at its evaporation or condensation in a mixture of vapors and non-condensable gas-carrier. The set is quite general because obtained balance equations together with the complete transport equations allow one to take accurately into account the non-stationary effects of diffusion [5], heat conduction [6,7], transient processes in the droplet before reaching the stationary concentration and composition [7,8], cross-effects of mutual and thermal diffusion, the Stefan flow and motion of the boundary of the droplet [5]. The solution in the droplet is considered to be non-ideal, and the effects of non-ideality on the partial volumes, evaporation and specific heats, saturation pressure of components are included [9]. Our analysis shows that a correct description of the thermal effects at condensational growth or evaporation of multicomponent droplets is only possible within the non-stationary approach to the heat and mass transfer in the vapor-gas environment. Under the condition that the concentrations of condensable vapors are much smaller than the concentration of passive gas, we simplified the set of equations to the case when the effects of non-stationary diffusion and thermal conductivity are considered, but the effects of thermal diffusion, the Stefan flow and the movement of the boundary of the droplet can be neglected. In the steady regime of growth or evaporation of a multicomponent droplet, the equations for the stationary values of temperature and component concentrations in the droplet have been derived and analyzed.

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