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Proper orthogonal decomposition (POD) analysis of flow structure in volatile binary droplets☆

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ABSTRACT

In the present study we perform an in-depth analysis of the internal flow induced by concentration gradients in an evaporating binary ethanol–water droplet. The flow structure during the first stage of evaporation is characterised using micro particle image velocimetry (PIV) to investigate the flow field and analyse various modes of convection. Although PIV shows convection vortices, it does not help in identifying the various superimposed convection modes present. The proper orthogonal decomposition (POD) method is hence used in conjunction with PIV data to identify and characterise prevailing convection modes. During the first stage of evaporation many modes i.e. flow structures are found to co-exist, however the analysis reveals one dominant mode. In addition to the identification of this new mode of convection, the analysis quantifies the energetic contribution of each of these convection modes. The dominant mode is found to contribute to more than half of the total kinetic energy.

1. Introduction

Because of growing interests in potential applications involving wetting and evaporation of droplets, the topic has recently seen a rapid expansion. The breadth of literature on the subject over the last two decades highlights the increase of the number of studies dedicated to understanding this seemingly simple yet fundamental process [1–9]. Most of the studies however have focused on investigating the behaviour of single component droplets. It is worth noting that many applications do involve either binary or multicomponent droplets. Combustion, crop dusting and reactive wetting are some examples where multicomponent droplets are encountered. This stresses the need for further studies of binary and multicomponent droplet wetting and evaporation behaviour. The internal flow structure within evaporating droplets and its evolution is one aspect which is of great importance to a better understanding of the phenomenon.

Recent studies have demonstrated the existence of various and distinct flow regimes during the evaporation of binary droplets [3–6]. Regardless of the initial concentration, the flow is characterised by the succession of three flow regimes [7]. A first stage where multi-vortices are observed and where the spatial averaged vorticity is roughly constant. A second stage, which is characterised by an exponential decline of vorticity intensity which represents the transition to a final third stage. This stage is dominated by an outward flow regime, this later being typical of pure component droplets. The three flow regimes have been analysed recently and interpreted in terms of the existence of different operating mechanisms such as solutal Marangoni effect driven by concentration gradients leading to multi-vortices observed during the first stage of evaporation [8]. The localised evaporation near the three-phase contact line and continuity cause an outward flow observed in the third and final stage of evaporation of binary aqueous droplets [9]. The second stage, characterised by the decline in vorticity is the result of depletion of the more volatile component and transition to a near pure water droplet. It is however realised that during the first stage of evaporation, many flow structures can coexist. Convection driven by solutal Marangoni mechanism and an outward flow resulting from mass conservation, are thought to be both present during the first stage. This combination of flow regimes leads to a rather complex flow structure in the first stage of evaporation which is worth further investigation.

Indeed, careful examination of the PIV data shows that the first stage is characterised by a transient flow where more than one mode of convection is present. Although the spatial averaged vorticity remains constant during the first stage, various modes and number of vortices are evolving in time. Characterising these flow modes and their relative prevalence can contribute to a better understanding of the

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phenomenon. The evolution of convection modes during the first stage of evaporation of an aqueous binary sessile droplet is therefore still an open question.

In the present letter we focus our attention on the first flow regime. This latter is characterised by a constant spatially averaged vorticity. We attempt to perform an in-depth analysis to reveal the dominant modes of convection. To this end we use a new approach that is proper orthogonal decomposition (POD) method [10] to analyse data obtained via micro-PIV. We also aim to quantify the energy contribution of the most significant convection modes.

2. Experiments and analysis

The details of the experimental setup and procedures can be found in references [7–9]. Ethanol–water binary droplets are deposited on transparent slides and a PIV analysis of the internal flow is performed. The flow is observed through the base of the droplet. Three stages of the internal flow as characterised by the PIV measurements are revealed. The full discussion of these stages can be found in [8], in the present study we use data for a 25% ethanol concentration. The first stage of evaporation, which is the focus of the present study, is characterised by multiple vortices believed to be induced and dominated by concentration gradients [8]. The PIV analysis shows that the averaged vorticity during this stage is fairly constant, Fig. 1. When examining the PIV data in more detail, it is observed however that the flow structure evolves and many modes of convection are superimposed, Fig. 2. The flow structure and its evolution during this first stage of evaporation is clearly complex in nature. It is obvious from PIV observations that there are multiple vortices as well as other flow structures which are evolving in time.

Another observation from the same PIV data is that in addition to the distinct vortices and convection rolls, there is another superimposed flow which is rather chaotic in nature. This flow is not easily characterised with the sole PIV data. In the sequence shown in Fig. 2, the number of vortices varies from three to six vortices. Careful examination of stream lines and velocity vectors, in Fig. 2, reveals a flow between and on top of these distinct convection rolls.

The PIV data shown in Fig. 2 clearly indicate the presence of more than one mode of convection. These modes evolve during the first stage of evaporation although the averaged vorticity remains fairly constant as discussed in [7,8].

It is clear from the PIV data that during the first stage of evaporation of these binary droplets, the flow structure is rather complex and evolving in time. The PIV data alone however do not allow an identification of dominant modes and their contribution to convective energy transport. Worth mentioning that the actual shapes of droplet bases deviate slightly from the circular form. The data in Fig. 2 have been cropped to focus on the flow and avoid edge effects.

3. The proper orthogonal decomposition (POD) approach

The proper orthogonal decomposition (POD) is widely used in literature, allowing identification of instantaneous and time varying flow structures. The POD technique decomposes the original field (vector or scalar) into a sum of weighted, linear, basis modes. The creation of the basis functions is a statistical correlation method with normalised and orthogonal basis functions. For velocity treatment, the POD is interesting because the optimization of the basis in *L2* space distinguishes and ranks the modes according to energy [11]. The POD needs input data composed of K two-dimensional velocity fields sampled in time, $Vk = (u_i^j, v_i^j)^k$ where, i, j are the indices of the grid points in the PIV measurement plane and k is the time index of the velocity field. The POD produces a linear basis set consisting of M basis functions ϕ_m and the corresponding coefficients c_m^k, that can reconstruct all K velocity distributions. Few modes are generally sufficient to reconstruct physical flow structures because each POD mode includes elements of all flow structures from the K input fields. The m is the index of the M mode deduced from the K field with $M = K$. The procedures of determining the orthonormal POD basis functions ϕ_m are detailed in [11–13].

As the basis functions ϕ_m are normalised, the velocity amplitude information is given by c_m^k. The corresponding kinetic energy per unit mass ($Ekin$) and total kinetic summed over all the K velocity fields ($Ekin_{Tot}$) are given respectively by:

$$Ekin_m = \sum_{k=1}^{K} \frac{1}{2} \left(c_m^k\right)^2 \tag{1}$$

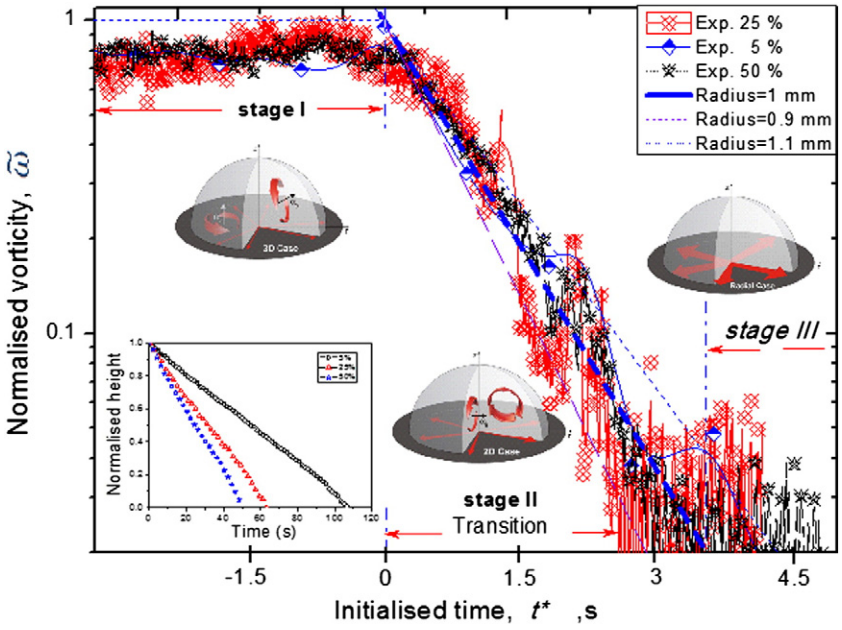

Fig. 1. Measured averaged and normalised vorticity for three difference initial ethanol concentrations, indicating three distinct successive stages in flow structure, see [8]. Inset figure represents the evolution of droplets height versus time.