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# ON SIMULATION OF CLOUDS AND FOGS CONDENSATION

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## Abstract

The expansion of Computer Algebra Systems (CAS) to mathematics-related fields of science such as physics, chemistry and biology is a trend of the last few years. This presentation is a short report devoted to our first results in using CAS DERIVE in surface colloid phenomena and mainly in presenting derived results in the form of mathematical movies with the help of the DERIVE + DPGraph + Hotkeys keystroke simulator complex we reported at the 5th ACDCA Summer Academy in August 1999 [1].

Water vapor condensation on chemically heterogeneous aerosol particles in the atmosphere is under consideration. This problem is important in current research on heterogeneous cloud and fog nucleation (microphysics of clouds), weather modification (artificial rain or precipitation of hail clouds), aerosol models for interpretation of data obtained from lidar systems monitoring air quality, and investigations of the aerosol effects on climate forcing.

## 1. Heterogeneous Surface Peculiarities (Theoretical Background)

As usual, all atmospheric “nuclei” of condensation (CN) or ice crystallization (IN) are the chemically mixed aerosol particles (MAP) having the energetically heterogeneous surface. An origin of the heterogeneity may be a result of natural physical-chemical processes, such as gas adsorption, photochemical surface reactions, aerosol coagulation etc. From the other hand, an artificial heterogenization of aerosol particles increases their ice-nucleating activity; this fact was used for weather modification through the silver iodide aerosol systems [2]. Some time ago researchers found different natural bioaerosols (in part, *Pseudomonas syringae*) in the atmosphere, wich is playing also a role of the effective ice-nucleating “nuclei” in cold clouds. Typically, a cell membrane surface built from phospholipids and trans-membrane proteins is heterogeneous.

From a viewpoint of water wetting one may distinguish between hydrophilic and hydrophobic solid surfaces. The hydrophilic ones with a low free surface energy, $\sigma$, have values of the contact angles of wetting in a range: $0^0 \le \theta < 90^0$, while the hydrophobic those with a high free surface energy the contact angles are in a range: $90^0 \le \theta \le 180^0$. Solid surfaces having both hydrophobic and hydrophilic sites are heterophilic. For some purposes there is conveniently to use a “heterophilic” term for surfaces having sites with different values of the contact angle only. A “heterogeneity” term includes both a surface roughness (topography) and the energetic non-homogeneity; dealing with heterophilic surfaces one may use the term “heterophilic” and “heterogeneous” as synonyms. Two important factors to be taken into account in the heterophilic surface analysis are the heterogeneity scale and the topology. A detailed analysis of main peculiarities of the heterophilic surfaces in phenomena of adsorption, wetting and condensation was given in a series of our works (see, e.g., [3]). First, new physical phenomena were discovered on MAPs: (1) a “double barrier

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nucleation" and (2) a "quasi-cavitational" mechanism of heterogeneous condensation [2-3]. We shall present a visual computer simulation of the double barrier nucleation phenomenon in this report.

## 2. Heterogeneous Condensation and Drop Evolution.

**A.** We shall consider a simple model of condensation on a spatially extended, isolated, hydrophilic ("active") site of radius $R_d$ (of macro- or "colloidal" scale: $R_d > 5$ nm) on a spherical aerosol particle (with a radius $R_0 \sim 1$ μm) with a wetting angle $\theta_i < \theta_0$ (where $\theta_0$ – is the characteristics of the surface surrounding the "active" site ). We assume that a liquid embryo with a finite contact angle forms at the "active" site by a heterogeneous nucleation mechanism. If a radius of the embryo, R << $R_0$ , for a simplicity, the particle surface may be regarded as a flat. The image of a droplet on a hydrophilic spot is in Fig.1.

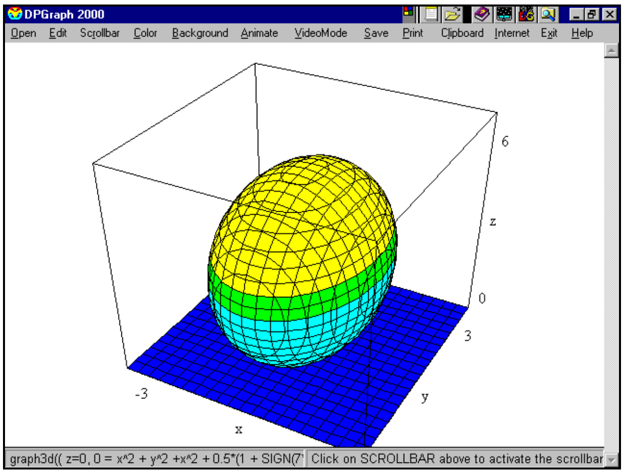


Fig.1. Growing droplet on the heterophilic substrate.

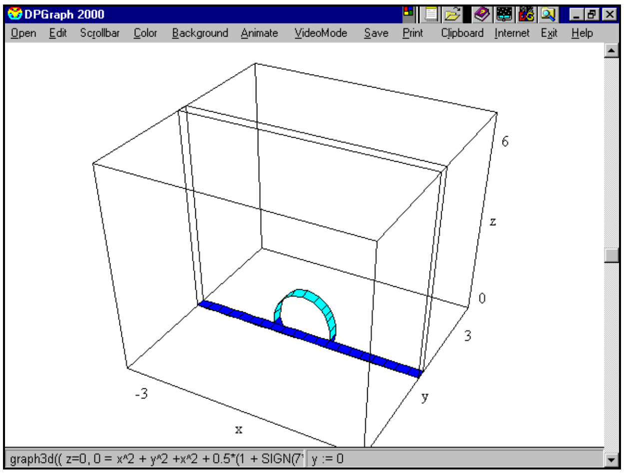


Fig.2. Small droplet on the hydrophilic spot.

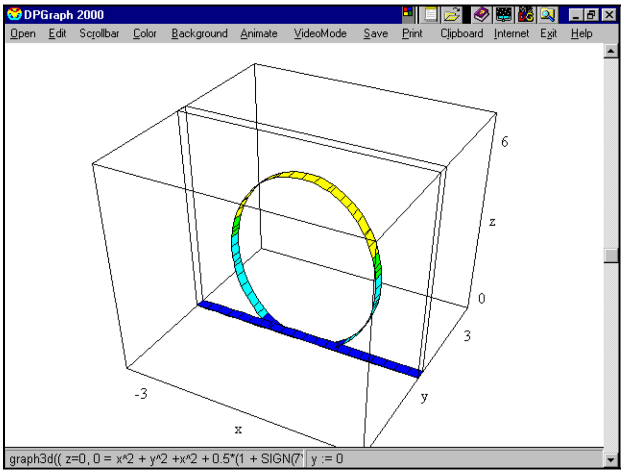


Fig.3. Big droplet on the hydrophilic spot.

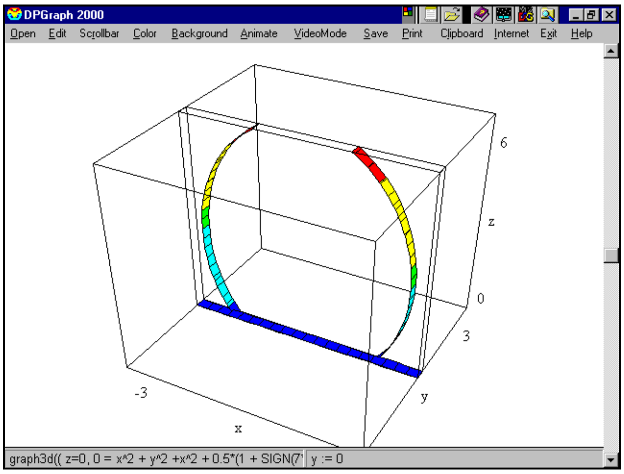


Fig.4. The droplet expansion on the hydrophobic substrate.

A droplet radius grows while its contact angle is constant ( $\theta = \theta_i = const$ , where $\theta_i$ is the Young's angle for the hydrophilic site). When a droplet reaches a boundary between the hydrophilic and hydrophobic sites, its perimeter is fixed (Fig.2). A droplet volume may grow if its radius increases and a variable contact angle, θ, increases to a critical value (Fig.3), where $\theta_0$ is a Young's angle for the hydrophobic surface. Then the droplet expands to the hydrophobic substrate (Fig.4). A study of Gibbs' free energy of the growing droplet as a function of its volume, using a variational analysis [2] shown an existence of two maxima (barriers) during a droplet nucleation and an evolution. Relative values of these barriers depends on a relationship between a critical nucleation radius and an "active" site radius, $R_d$. The above figures are screenshots of a 3D movie in DPGraph produced with the help of DERIVE and Hotkeys [1]. The appropriate rotation and adjustment of figures 2-3 results in 2D movies.

**B.** A model of a droplet at an insoluble spherical aerosol particle with hydrophilic surface with two hydrophobic sites on its poles was regarded in [3,5]. As it was found, in beginning of the condensational growth a liquid phase covers only hydrophilic sites and the hyrophobic spot is free of water (Fig.5,6,8); then, at some critical volume, one of holes collapses and only a small air-vapor hemisphere bubble covers hydrophobic spot (Fig.7). This process provokes the "surface-cavitation" mechanism of the fast secondary condensation [3]. The movie of the process is also presented.

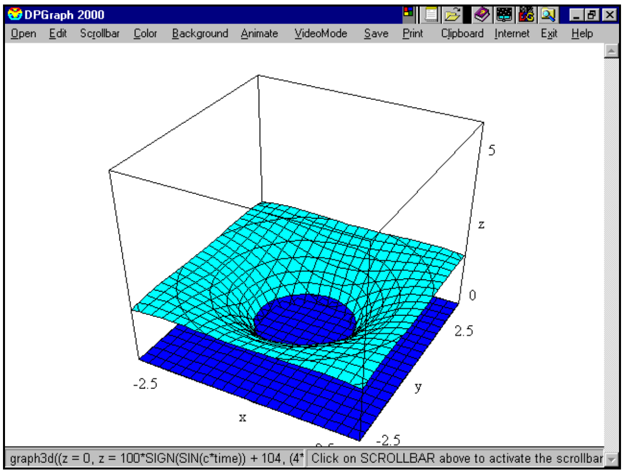


Fig.5. Hydrophobic spot on a hydrophilic substrate is not covered with a thin water film.

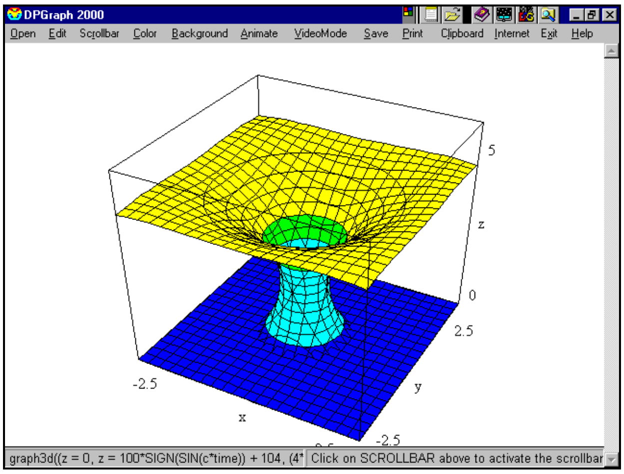


Fig.5. The same as in Fig.5, but thicker water film.

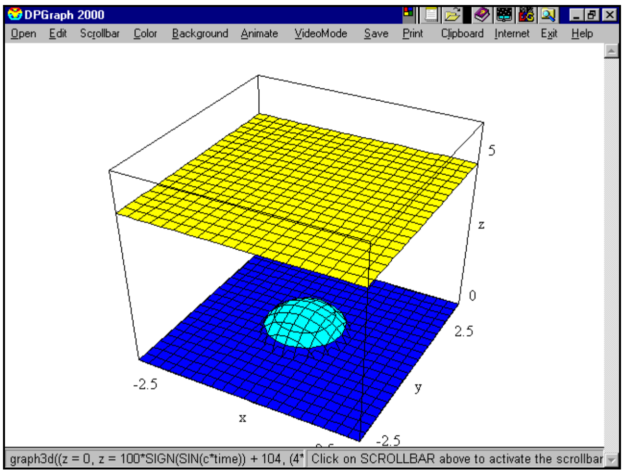


Fig.7. More thick water film. The hole in water film collapsed and a small air bubble remained.

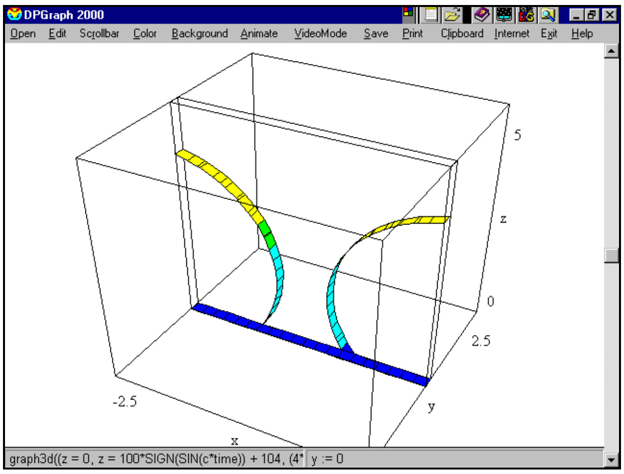


Fig.8. 2D section of Fig.6 - the hole shape.

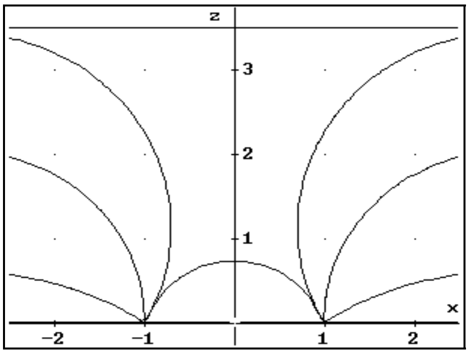


Fig.9. Successive air-water bounds for “surface cavitation” (DERIVE)

All above figures were 3D screenshots from DPGraph movies. It is colorful, animated and clear to undestand and percept at the display, but rather difficult to be adequatly presented in the black and white printed form. Static 2D images better corresponds the printed form of presentation and can be easily made in DERIVE. Fig. 9 shows the above “surface-cavitation” as a set of sequantial in time surfaces air-water 2D sections.

### 3. Phenomena of Heterogeneous Evaporating of Drop and Capillary-Hydrodynamic Instability of Wetting Film

During a drop evaporation from an insoluble aerosol particle, a thinning liquid layer will be transformed into separated liquid clusters at some critical thickness, due to fluctuational-hydrodynamic surface waves. A wave mode of the fastest grow which leads to the film rupture, may be regarded as an “anti-soliton”. Theoretical background of the phenomenon is discussed in [4-5]. The “anti-soliton” propagation leading to the film rupture is demonstrated in a form of the 3D-math movie in Fig.10, 11. The left image is similar to the inverse tsunami at the shallow water [1]. The right one - water film rupture and two thin separate scattering films opening the hydrophobic surface.

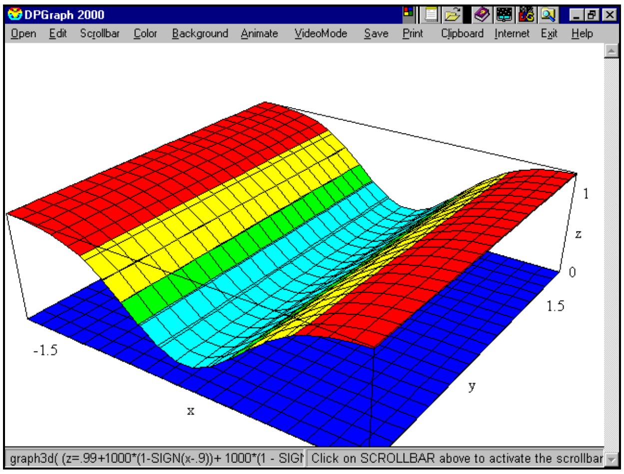


Fig.10. Surface “anti-soliton” wave.

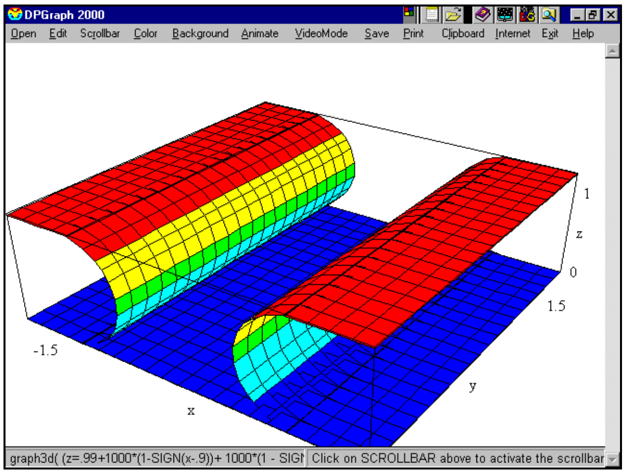


Fig.11. Film rupture.

As it was shown in [5], during condensation-evaporation cycle in atmosphere of aerosol hazes or fogs, regarded above phenomena give us an explanation of an effect of the hysteresis dependence of the light-scattering coefficient on relative humidity for cases of insoluble aerosol particles. Our concept complements a convenient approach developed for soluble condensational “nuclei” and used in lidar monitoring programs of air quality [6].

## References

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