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Three-Dimensional Computer Simulation of Liquid Drop Evaporation

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Abstract—We use molecular dynamics simulation to describe a method that can be used to model liquid drop evaporation. For application, the liquid is taken to be water. Using the properties of the liquid and a Lennard-Jones potential, we derive dynamical equations, which are used to describe the gross dynamical behavior of the liquid-vapor molecular system. The resulting dynamical equations are solved numerically by a time stepping, numerical method. The evaporation of the liquid to the vapor phase is described. © 2000 Elsevier Science Ltd. All rights reserved.

Keywords—Liquid drop, Evaporation, Molecular model.

1. INTRODUCTION

Mathematicians, engineers, and scientists have shown a broad interest in fluid drops (see, e.g., [1–6], and the references contained therein). Even though many of the modern studies of fluids use the continuum approach, it is an accepted fact that the molecules or atoms in fluids play a fundamental role in fluid phenomena.

Water evaporation is essential in meteorological studies, and in the prediction of liquid-fueled combustor performance and stability, knowledge of droplet lifetimes is essential.

The nature of matter is to be found in the structure and motion of its constituent building blocks—atoms or molecules [7]. In particular, the gross dynamical behavior of any fluid is determined by the behavior of these constituents. In general, the number of atoms or molecules is so large as to prohibit the determination of the behavior of each atom or molecule. This motivated the development and application of statistical mechanics, which combines the rules of statistics with the laws of Newtonian mechanics to describe quantitative large scale properties of solids and fluids from the most probable behavior of their constituent building blocks [7–11]. The development of modern computers has led to molecular dynamics simulation, in which one simulates the motion of a small subset of the atoms or molecules with the expectation of deriving or verifying results that are applicable in the large [12–14]. However, in view of the current interest in nanotechnology, molecular dynamics simulations are of interest in themselves.

The molecular dynamics method is computationally demanding, but since it attempts to mimic nature, it has few inherent limitations. An advantage is that all attendant physical phenomena,

viscosity, surface tension, evaporation, condensation, etc., come from the intermolecular potential function.

Two-phase behavior for liquid drops has been previously simulated (see [15–17], and the references contained therein). However, with only one exception [17], which discussed liquid argon droplet evaporation, these simulations dealt with other properties of fluids—density, surface tension, and thermodynamics properties.

Water is the only known substance that commonly exists in all three phases (solid, liquid, and gas) at once. The speed of each water molecule determines that molecule's phase. In particular, from the kinetic theory of gases, the speeds of water molecules determine condensation and evaporation rates.

In this paper, we simulate water drop evaporation at the molecular level. From the potential function between two water molecules, the local force of interaction between them will be derived, followed by the dynamical equations of the drop molecular system. The resulting system of dynamical equations must be solved numerically since it lacks a general analytical solution.

2. EQUATIONS OF MOTION

From the classical Newtonian point of view, the interactions between pairs of atoms in close proximity to each other are responsible for providing the two principal features of an intermolecular force [7]. The first is a resistance to compression; hence, the molecules repel at close range. The second is to bind the molecules together in the solid and liquid states; and for this, the molecules attract each other over a range of separations. Potential functions exhibiting these characteristics can adopt a variety of forms. The best known of these potential functions, originally proposed for liquid argon, is the Lennard-Jones potential [18]. The Lennard-Jones 6-12 potential for a pair of atoms or molecules P_i and P_j located at \vec{r}_i and \vec{r}_j , respectively, is

$$\phi(r_{ij}) = \begin{cases} 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right], & r_{ij} \leq r_c, \\ 0, & r_{ij} > r_c, \end{cases} \quad (1)$$

where $\vec{r}_{ij} = \vec{r}_j - \vec{r}_i$ and $r_{ij} = \|\vec{r}_{ij}\|$. The parameter ε is the minimum potential energy and σ is the zero potential energy separation distance. The interaction repels at close range, then attracts, and eventually it is cut off at some limiting separation r_c .

The force associated with $\phi(r)$ is $f = -\frac{\partial\phi(r)}{\partial r}$ and is directed along the line connecting the atoms or molecules. Thus, the force of interaction between two atoms or molecules P_i and P_j , located at \vec{r}_i and \vec{r}_j , respectively, corresponding to the potential function in (1) is obtained from the equation

$$\vec{f}(r_{ij}) = \begin{cases} -\frac{\partial\phi(r_{ij})}{\partial r_{ij}} \frac{\vec{r}_{ji}}{r_{ij}}, & r_{ij} \leq r_c, \\ 0, & r_{ij} > r_c. \end{cases} \quad (2)$$

A graph of $\phi(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6]$ is shown in Figure 1. Notice from Figure 1 that the two atoms or molecules experience a significant attractive force when the separation distance r is in the range 1.1σ – 2σ . The force is essentially zero for separations larger than 3σ , while for $r \leq 1.1\sigma$, the force is strongly repulsive.

The equations of motion follows from Newton's second law of motion

$$m\vec{\ddot{r}}_i = \vec{f}_i, \quad (3)$$

where \vec{f}_i is the force on P_i , m is the mass of P_i , \vec{r}_i is the position vector of P_i , and differentiation is with respect to time. Since the molecular interaction during the liquid drop evaporation is

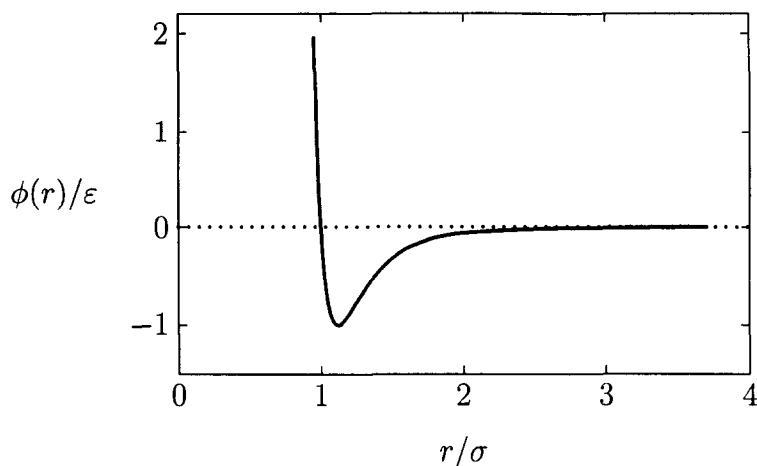


Figure 1. Lennard-Jones 6-12 potential.

independent of gravity, we neglect long-range forces. Thus, it follows from (3) that the equations of motion are of the form

$$m\ddot{\vec{r}}_i = \sum_{\substack{j=1 \\ j \neq i}}^N \vec{f}(r_{ij}), \quad i = 1, 2, \dots, N, \quad (4)$$

where the summation is over all N molecules, excluding P_i , and $\vec{f}(r_{ij})$ is the force that molecule j exerts on molecule i .

Substituting $\epsilon = (4.9115)10^{-14}$ and $\sigma = 2.725$ into (1), we obtain an approximate Lennard-Jones potential for two water molecules, P_i and P_j , r_{ij} angstroms (\AA) apart, given by [18]

$$\phi(r_{ij}) = (1.9646) 10^{-13} \left[\left(\frac{2.725}{r_{ij}} \right)^{12} - \left(\frac{2.725}{r_{ij}} \right)^6 \right] \text{erg}. \quad (5)$$

Since $1 \text{ cm} = 10^8 \text{ \AA}$, it follows that for R_{ij} measured in cm, $r_{ij} = 10^8 R_{ij} \text{ \AA}$. Thus, from (5), the force \vec{F} on P_i due to P_j is given by

$$\begin{aligned} \vec{F}(r_{ij}) &= -\frac{d\phi(r_{ij})}{dR_{ij}} \frac{\vec{R}_{ji}}{R_{ij}} \\ &= -\frac{d\phi(r_{ij})}{dr_{ij}} \frac{dr_{ij}}{dR_{ij}} \frac{\vec{R}_{ji}}{R_{ij}} \\ &= -10^8 \frac{d\phi(r_{ij})}{dr_{ij}} \frac{\vec{r}_{ji}}{r_{ij}} \text{ dynes.} \end{aligned}$$

Thus,

$$\vec{F}(r_{ij}) = (4.8264) 10^{-2} \left(\frac{818.9}{r_{ij}^{13}} - \frac{1}{r_{ij}^7} \right) \frac{\vec{r}_{ji}}{r_{ij}} \text{ dynes}, \quad (6)$$

$F(3.059) = 0$. Thus, $\bar{r} = 3.059 \text{ \AA}$ is the equilibrium distance of separation between two neighboring water molecules.

Because of the nature of the intermolecular interaction exemplified by the Lennard-Jones potential with a strong repulsive component, molecular trajectories are unstable in the sense that an infinitesimal perturbation will grow at an exponential rate.

The mass of a water molecule is $m = (30.103)10^{-24} \text{ g}$. From (4), a dynamical equation of a water molecule P_i as it interacts with other water molecules is given by

$$m \frac{d^2 \vec{r}_i}{dt^2} = \sum_{\substack{j=1 \\ j \neq i}}^N \vec{F}(r_{ij}). \quad (7)$$

Substituting for m and using equation (6), equation (7) becomes

$$\frac{d^2\vec{r}_i}{dt^2} = \sum_{\substack{j=1 \\ j \neq i}}^N (1.6033)10^{21} \left(\frac{818.9}{r_{ij}^{13}} - \frac{1}{r_{ij}^7} \right) \frac{\vec{r}_{ji}}{r_{ij}} \frac{\text{cm}}{\text{s}^2}. \quad (8)$$

Changing to $\text{\AA}/\text{s}^2$, equation (8) yields

$$\frac{d^2\vec{r}_i}{dt^2} = \sum_{\substack{j=1 \\ j \neq i}}^N (1.6033)10^{29} \left(\frac{818.9}{r_{ij}^{13}} - \frac{1}{r_{ij}^7} \right) \frac{\vec{r}_{ji}}{r_{ij}} \frac{\text{\AA}}{\text{s}^2}. \quad (9)$$

We now use the computationally convenient time transformation $T = 10^{12}t$, which leads to a time measurement in picoseconds ($1 \text{ s} = 10^{12} \text{ ps}$), where ps represents picosecond. Thus, equation (9) becomes

$$\frac{d^2\vec{r}_i}{dT^2} = \sum_{\substack{j=1 \\ j \neq i}}^N (1.6033)10^5 \left(\frac{818.9}{r_{ij}^{13}} - \frac{1}{r_{ij}^7} \right) \frac{\vec{r}_{ji}}{r_{ij}} \frac{\text{\AA}}{\text{ps}^2}, \quad (10)$$

which will be used in actual computation.

From given initial data, the motion of each water molecule P_i is determined by solving the system of second-order, nonlinear, ordinary differential equations in (10) using the leap frog numerical method [19]. Throughout the unit for length is the angstrom, and that for time is the picosecond. And, as usual, $T_k = k\Delta T$, $k = 0, 1, 2, \dots$

3. INITIAL DATA GENERATION AND MODEL

Consider a regular tetrahedron with edge length r . Its altitude is $a = \sqrt{2/3} r$. Using these values, we construct a regular tetrahedral grid as follows:

$$\begin{aligned} x_1(1) &= -9r, & y_1(1) &= -5\sqrt{3} r, & x_1(20) &= x_1(1) + 0.5r, & y_1(20) &= y_1(1) + \left(\frac{\sqrt{3}}{2}\right)r, \\ x_1(i) &= x_1(i-1) + r, & y_1(i) &= y_1(1), & & & i &= 2, 3, \dots, 19, \\ x_1(i) &= x_1(i-1) + r, & y_1(i) &= y_1(20), & & & i &= 21, 22, \dots, 37, \\ x_1(i) &= x_1(i-37), & y_1(i) &= y_1(i-37) + \sqrt{3} r, & & & i &= 38, 39, \dots, 389, \\ x_2(1) &= x_1(1) + 0.5r, & y_2(1) &= y_1(1) + \left(\frac{\sqrt{3}}{6}\right)r, \\ x_2(19) &= x_1(1), & y_2(19) &= y_1(1) + \left(\frac{2\sqrt{3}}{3}\right)r, \\ x_2(i) &= x_2(i-1) + r, & y_2(i) &= y_2(1), & & & i &= 2, 3, \dots, 18, \\ x_2(i) &= x_2(i-1) + r, & y_2(i) &= y_2(19), & & & i &= 20, 21, \dots, 37, \\ x_2(i) &= x_2(i-37), & y_2(i) &= y_2(i-37) + \sqrt{3} r, & & & i &= 38, 39, \dots, 370. \end{aligned}$$

The above algorithm generates two layers of points. The set of points $(x_1(i), y_1(i))$, $i = 1, 2, \dots, 389$ generates layer one, and that of $(x_2(i), y_2(i))$, $i = 1, 2, \dots, 370$ generates layer two.

We arrange the above layers of points alternately beginning with layer one as follows.

$$\begin{aligned} k &= 0, h = -6a \\ \text{For } j &= 1 \text{ to } 7 \text{ do} \\ &\quad \text{For } i = 1 \text{ to } 389 \text{ do} \end{aligned}$$

```

    k = k + 1, x(k) = x1(i), y(k) = y1(i), z(k) = h
End loop
h = h + a
For i = 1 to 370 do
    k = k + 1, x(k) = x2(i), y(k) = y2(i), z(k) = h
End loop
h = h + a
End loop
For i = 1 to 389 do
    k = k + 1, x(k) = x1(i), y(k) = y1(i), z(k) = h
End loop

```

This arrangement yields a set of points in 3D arranged at the vertices of a regular tetrahedral grid of edge length r .

Setting $r = 3.1 \text{ \AA}$ and taking only points satisfying $x(i)^2 + y(i)^2 + z(i)^2 \leq 17^2$, we get a spherical configuration of 955 points. We place water molecules at these points to get a relatively spherical water drop with radius 17 \AA and consisting of 955 water molecules. Notice that, rounded to one decimal position, the equilibrium distance of separation ($\bar{r} = 3.059$) between two water molecules, obtained from equation (6), is 3.1 \AA .

Similarly, we set $r = 15.5 \text{ \AA}$ in the above algorithm to generate points at the vertices of a regular tetrahedral grid, and take only the points satisfying $|x(i)| \leq 4.5r$, $|y(i)| \leq 4.5r$, $|z(i)| \leq 4.5r$, and $x(i)^2 + y(i)^2 + z(i)^2 > 17^2$. We place water vapor molecules at these points to get 1082 water vapor molecules.

Plotting the water and vapor molecules generated above on the same graph, we get a spherical water drop centered at the origin and surrounded by water vapor molecules. A top view of the resulting configuration is shown in Figure 2, which consists of a water drop embedded in water vapor molecules in a cube of edge length 139.5 \AA centered at the origin. The dark cluster at the center of Figure 2 is the water drop surrounded by water vapor molecules. The total number of molecules in Figure 2 is 2037. Notice that the vapor molecules are relatively far apart, and that inside the water drop, the molecules are packed closely together. That is, in the liquid, the molecules are denser than those in the vapor region, as expected.

From the kinetic theory of gases, temperature is a direct measure of average molecular kinetic energy; the average (root mean square) speed of the molecules is given by [7]

$$v = \sqrt{\frac{3kT}{m} \frac{\text{cm}}{\text{s}}}, \quad (11)$$

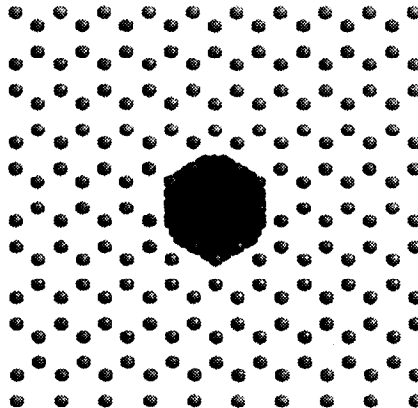


Figure 2. Initial water drop with surrounding water vapor molecules.

where m = mass of a single molecule, $k = (1.381)10^{-16}$ erg/kelvin (Boltzmann's constant), and T = temperature measured in kelvin. There are only three translational degrees of freedom for the molecules; therefore, the kinetic energy is purely translational and temperature is directly proportional to kinetic energy. From (11), we get

$$v = 0.370981772\sqrt{T_c + 273} \frac{\text{\AA}}{\text{ps}}, \quad (12)$$

in which T_c is temperature measured in degrees centigrade. Using (12), we set the temperatures of the water molecules and the vapor molecules to 15°C and 100°C , respectively. This is done by using (12) to get the speed of the molecules corresponding to the temperature and then using it to assign initial velocities to the molecules in random directions. In each case, water molecules or water vapor molecules, the velocities are set to a fixed value that depends on the temperature, and after assignment of random velocity directions, the velocities are adjusted to ensure that the center of mass is stationary.

4. RESULTS

With the above initial data (initial positions and velocities) set, we begin the simulation by first stabilizing the initial configuration in Figure 2. We choose $\Delta T = 0.0001$ and $r_c = 17 \text{\AA}$. The time step is chosen to be very small in order to avoid errors and for physical stability of the molecular system. Notice that $r_c \approx 6.238\sigma$. The rationale for choosing $r_c = 17 \text{\AA}$ is to ensure one local distance of interaction between two neighboring vapor molecules of the initial configuration in Figure 2. We allow the molecules to interact in accordance with (10) and the leap frog numerical method.

The system of molecules is first allowed to interact for 20000 time steps; during this time period, the vapor molecules' velocities are restricted at each time step as follows. Let $\vec{v}_{i,k}$ denotes the velocity of vapor molecule P_i at time T_k . If $\|\vec{v}_{i,k}\| < 7.165 \text{\AA}/\text{ps}$ (speed corresponding to 100°C), $\vec{v}_{i,k}$ is reset to $\vec{v}_{i,k-1}$. At the end of the 20000 time steps, the restriction on the vapor velocities is removed and the molecules are allowed to interact to 35000 time steps. At this point, velocities whose magnitudes are greater than $10.0 \text{\AA}/\text{ps}$ are then rescaled to the speed $7.165 \text{\AA}/\text{ps}$, and the molecules allowed to interact further with no restriction on the velocities to 40000 time steps.

During the stabilization process, if a molecule leaves the box, it is reflected symmetrically back into the box. The resulting relatively stable initial water-vapor equilibrium configuration is shown in Figure 3, where we have translated the center of mass of the water drop cluster to the center of the simulation region and adjusted the surrounding vapor molecules appropriately.

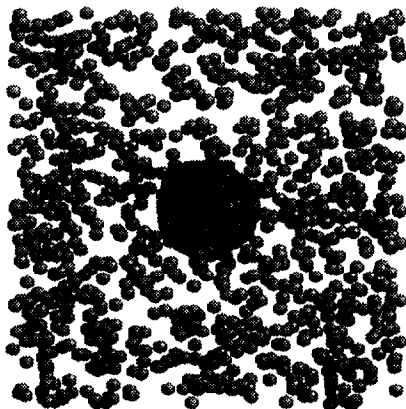


Figure 3. Stable water-vapor configuration (with 971 molecules in water drop).

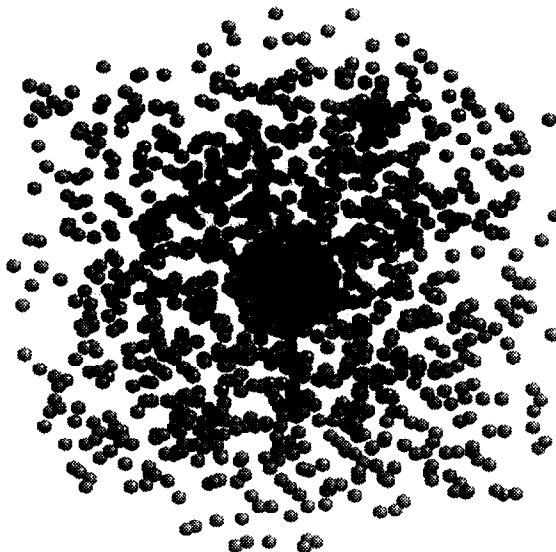


Figure 4. Stable water-vapor configuration viewed at an angle (with 971 molecules in water drop).

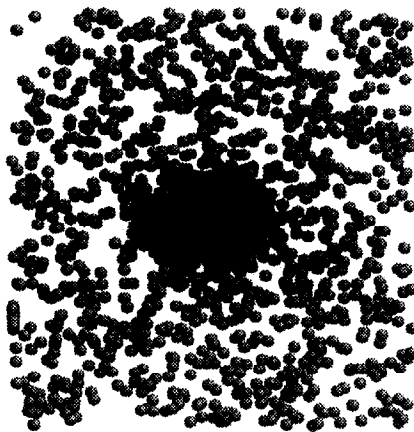


Figure 5. Evaporating water drop after 100000 time steps (888 molecules in water drop).

Throughout the simulation, the liquid drop is identified by finding the largest cluster among the molecules using the method of Stoddard [20]. In this regard, an exclusive search is performed over all possible pairs of molecules. A molecule P_j is identified to be associated with another molecule P_i in a cluster if $\|\vec{r}_i - \vec{r}_j\| < r_{cl}$, where r_{cl} is the classifying critical separation. We use $r_{cl} = 1.542\sigma$, as recommended by Thompson *et al.* [16]. The distance r_{cl} must be chosen to be sufficiently large to include the liquid drop, but not so large as to include all the molecules in the system. Thompson *et al.* showed in [16] that there is a range of r_{cl} values, independent of the size of the system, over which N_d (number of molecules in the drop at time t) remains constant. The r_{cl} value (1.542σ) used in this paper was chosen from such a range.

For the evaporation simulation, we use periodic boundary conditions throughout. There are two consequences of this periodicity. First, a molecule that leaves the cube through a particular bounding face immediately reenters the cube through the opposite face. Second, a molecule lying within a distance r_c of a boundary interacts with molecules in an adjacent copy of the system; that is, it interacts with molecules near the opposite boundary—a wraparound effect.

We begin with Figure 3 as the initial setting for the liquid drop evaporation, and use (10) along with the leap frog method. We use $\Delta T = 0.001$. Throughout, the evaporation is simulated

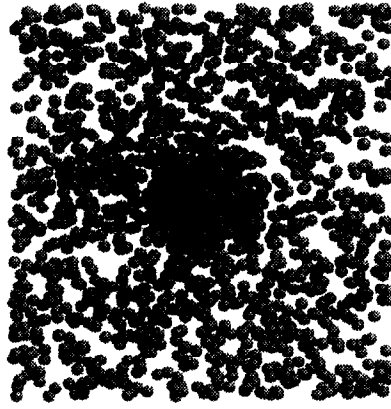


Figure 6. Evaporating water drop after 150000 time steps (549 molecules in water drop).

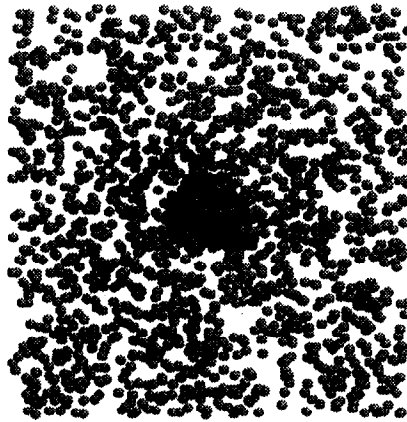


Figure 7. Evaporating water drop after 175000 time steps (353 molecules in water drop).

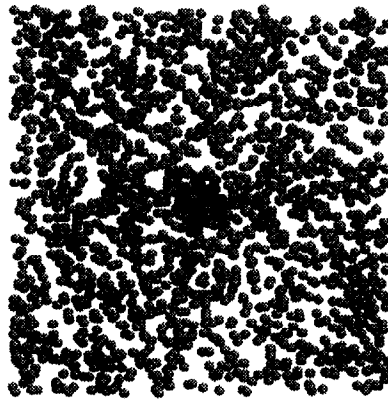


Figure 8. Evaporating water drop after 225000 time steps (56 molecules in water drop).

by heating the water vapors around the water drop in the boundary region of the cube. This is done by scaling the velocities of the vapor molecules in the region of the cube described by $50 < |x_i| \leq 69.75$, $50 < |y_i| \leq 69.75$, $50 < |z_i| \leq 69.75$ to a prescribed temperature after every 200 time steps. Of course, $\vec{r}_i = (x_i, y_i, z_i)$ is the position vector of molecule P_i . The location of the water drop as well as the surrounding water vapor molecules are adjusted after every 5000 time steps to offset the Brownian motion and also, most importantly, to prevent the water drop

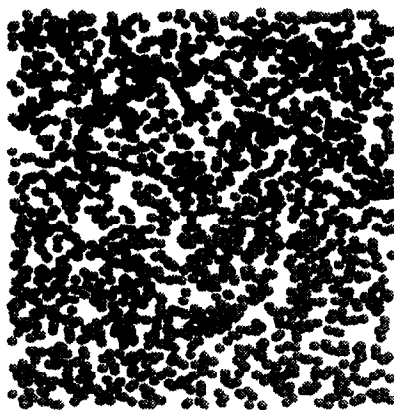


Figure 9. Evaporating water drop after 250000 time steps (three molecules in water drop).

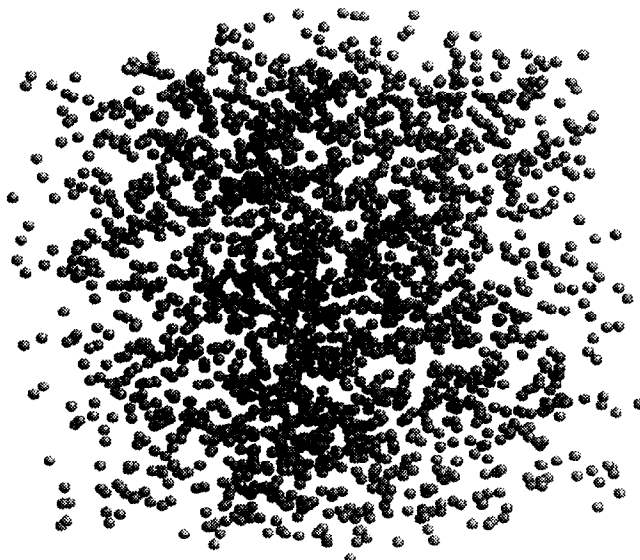


Figure 10. Evaporating water drop after 250000 time steps view at an angle (three molecules in water drop).

from entering the heating region. This is done by computing the center of mass of the liquid drop at time T_k ,

$$\vec{r}_{cm}(T_k) = \frac{1}{N_d} \sum_{i=1}^{N_d} \vec{r}_i(T_k),$$

and subtracting it from the position vector of each molecule (both water and vapor molecules). The result is a translation of \vec{r}_{cm} to the center of the cube. After each translation, the positions of the molecules are adjusted using periodic boundary conditions. The results obtained are shown in Figures 4–10, which show the evaporation of the water drop. For these results, we chose the speed $14 \text{ \AA}/\text{ps}$ as the speed of the molecules in the heating region after every 200 time step throughout the simulation.

5. REMARKS

The data for the simulation are outputs from programs run on a Pentium II 400 MHz PC. It required extensive computation. Increasing the number of molecules involved in the simulation, say, to 5000, would yield more accurate results and esthetic pictures, but this would require at present extensive supercomputation.

In addition to the results shown above, other cases were considered by varying the amount of heat in the heating region. We observed that evaporation and condensation were taking

place in all cases and that the speeds (and hence, the temperature) of the molecules determine condensation and evaporation rates. When the speed of vapor molecules in the heating region was lower, say to $10 \text{ \AA}/\text{ps}$, the evaporation rate was substantially reduced. On the other hand, when the speed of the vapor molecules in the heating region was further lower to a critical speed of $8 \text{ \AA}/\text{ps}$, condensation began to dominate; the number of molecules in the largest cluster began to increase during the simulation.

The above results agree qualitatively with experimental results on liquid drop evaporation. There are condensation and evaporation taking place during the simulation, and a liquid drop evaporates when evaporation dominates condensation.

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