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OF THE THREE DIMENSIONAL CAVITY
PROBLEM**

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MOLECULAR MECHANICS SIMULATIONS OF THE THREE DIMENSIONAL CAVITY PROBLEM

by

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1. Introduction.

The rapid development of computer technology has resulted in broad interest in three dimensional fluid simulation, which is known to have more complex force interactions than occur in two dimensions (see, e.g., refs. [1-6], [9], [11-15], [17], [18] and the additional references therein). In this paper we develop and analyze some molecular mechanics simulations of the three dimensional cavity problem. The fluid considered is water at 15° C.

2. Molecular Arrangement and Equations.

For two water molecules P_i and P_j which are r_{ij} Å apart, an approximate Lennard-Jones potential [8] is

$$(2.1) \quad \phi(r_{ij}) = (1.9646)10^{-13} \left[\frac{(2.725)^{12}}{r_{ij}^{12}} - \frac{(2.725)^6}{r_{ij}^6} \right] \text{ erg } \left(\frac{gr \text{ cm}^2}{sec^2} \right).$$

From (2.1), the force $\vec{F}_{ij}$ exerted on P_i by P_j is

$$(2.2) \quad \vec{F}_{ij} = (1.9646)10^{-5} \left[\frac{12(2.725)^{12}}{r_{ij}^{13}} - \frac{6(2.725)^6}{r_{ij}^7} \right] \frac{\vec{r}_{ji}}{r_{ij}} \text{ dynes } \left(\frac{gr \text{ cm}}{sec^2} \right).$$

Since the mass m of a water molecule is $(30.103)10^{-24}$ gr, equation (2.2) can be simplified to

$$\vec{a}_i = (160.33)10^{19} \left[\frac{818.90}{r_{ij}^{13}} - \frac{1}{r_{ij}^7} \right] \frac{\vec{r}_{ji}}{r_{ij}} \left(\frac{cm}{sec^2} \right).$$

For computational convenience the latter equation is cast finally in Å/ps²
(1 sec = 10¹² ps, 1 cm = 10⁸ Å) as

$$(2.3) \quad \vec{a}_i = (160330.) \left[\frac{818.90}{r_{ij}^{13}} - \frac{1}{r_{ij}^7} \right] \frac{\vec{r}_{ji}}{r_{ij}} \left(\frac{\text{Å}}{ps^2} \right).$$

The effective force on P_i is not determined by all molecules present, but primarily by those within an interactive distance D , which will be determined by

$$\frac{dF_{ij}}{dr_{ij}} = 0,$$

in which F_{ij} is the magnitude of $\vec{F}_{ij}$. The solution of this equation yields $r_{ij} = 3.39$ Å. Thus, for $r_{ij} \geq D = 3.39$ Å, we choose $\vec{F}_{ij} = \vec{0}$. From (2.3), then, the dynamical equation of a molecule P_i will be, for $r_{ij} < D$,

$$(2.4) \quad \vec{a}_i = (160330.) \sum_{\substack{j \\ i \neq j}} \left[\frac{818.90}{r_{ij}^{13}} - \frac{1}{r_{ij}^7} \right] \frac{\vec{r}_{ji}}{r_{ij}} \left(\frac{\text{Å}}{ps^2} \right).$$

Next, note that $F_{ij} = 0$ implies $r_{ij} = 3.06$ Å. Using this value we now construct a cubic grid of points as follows. Consider the three dimensional cube with

$$-52.02 \leq x \leq 52.02, 0 \leq y \leq 104.04, 0 \leq z \leq 104.04$$

as shown in Figure 1. The edge of this cube has length 104.04 Å and it is symmetrical about the YZ plane, that is, about the plane $x = 0$. In this cube our three dimensional cubic grid is constructed in the usual fashion with $\Delta x = \Delta y = \Delta z = 3.06$ Å, which results in 42875 grid points. Of these, 1225 points lie in the YZ plane and have x coordinate zero. At each grid point set a water molecule P_i ; $i=1,42875$. To complete the initial data for the molecules, note that at 15° C and at one atmosphere of pressure, the rms speed in Å/ps for a water molecule [10] is 6.3 Å/ps. This speed is assigned to each molecule in the X , Y , or Z direction, at random, but with the strong restriction that if P_i and P_j are not in the YZ plane, but are symmetrical relative to the YZ plane, then

$$V_x(P_i) = -V_x(P_j), V_y(P_i) = V_y(P_j), V_z(P_i) = V_z(P_j).$$

In this fashion, the flows to be studied will be amenable to personal computer simulation through the use of symmetry relative to the YZ plane [11], and the dynamics is reduced to a 22050-body problem.

For the 42875 water molecules with dynamical equations (2.4) and the initial data described above, we turn next to the following three dimensional cavity, or, basin, problem. The top face of the cube is the only face allowed to move. It moves in the Y direction and is allowed an extended length so that the fluid is always enclosed by six faces. The constant speed V of the top face is called the wall speed. Our problem is to describe the gross fluid motion within the cube for various values of V .

3. Computational Considerations.

The cavity problem will be solved numerically with the leap frog formulas [7] on a Digital Alpha 533 personal computer. For any time step Δt (ps) and $t_k = k\Delta t$, two problems must be considered. The first problem is to describe a protocol when, computationally, a molecule has crossed a face into the exterior of the cavity. For each of the lower five faces, we proceed as follows. The position will be reflected back symmetrically relative to the face into the interior of the cavity, the velocity components tangent to the face will be set to zero, and the velocity components perpendicular to the face will be multiplied by -1 . If the molecule crosses the moving face, then its position will be reflected back symmetrically, its x component of velocity will be set to zero, its z component of velocity will be multiplied by -1 , and its y component of velocity will be increased by the wall speed V .

Our next problem derives from the fact that an instantaneous velocity field for molecular motion is Brownian. In order to better interpret gross fluid motion, we introduce average velocities as follows. For J a positive integer, let particle P_i be at $(x(i, k), y(i, k), z(i, k))$ at $t_k = k\Delta t$ and at $(x(i, k-J), y(i, k-J), z(i, k-J))$ at $t_{k-J} = (k-J)\Delta t$. Then the average velocity $\vec{v}(i, k, J)$ of P_i at t_k is defined by

$$\vec{v}_{i,k,J} = \left(\frac{x(i,k)-x(i,k-J)}{J\Delta t}, \frac{y(i,k)-y(i,k-J)}{J\Delta t}, \frac{z(i,k)-z(i,k-J)}{J\Delta t} \right).$$

In the examples to be discussed, we will describe results for various choices of J .

4. Examples.

Consider first $V = 25$, $\Delta t = 0.00008$, and $J = 25200$. Figures 2-6 show vortex development for $x = 0$, that is, in the YZ , plane at the respective times $t = 2.90, 3.35, 4.02, 7.04, 10.07$. Figure 2 reveals the development of a compression wave moving down and to the left. This results in compression and molecular repulsion upwards, as is apparent in the upper left sections of Figures 3 and 4. Continuation of this motion results in the vortex flows shown in Figures 5 and 6. The mean speed in Figure 6 at 10.07 is 9.46 Å/ps. For graphical clarity, the velocities are reduced by the factor $v_m = 0.51$ in Figures 2-6.

Calculations using $J = 19600, 22400, 28000, 30800$ yielded results entirely similar to those displayed in Figures 2-6.

Motion of molecules not in the YZ plane was often difficult to display. Those to be described next were for the time interval $0 \leq t \leq 8.912$ ps. It is important in these examples to be aware of the units on the axes in each figure.

The molecule P_{17000} , labelled A in Figure 7, is at $(-3.06, 58.14, 87.68)$ initially. After extensive local interaction, the molecule moves to $(-2.21, 33.61, 81.35)$, which is labelled B in Figure 7. It then moves rapidly in the Z direction to $(-2.42, 24.23, 100.32)$, labelled C in the figure. Both X and Y values change rapidly next as the molecule moves to the point $(-17.24, 38.61, 102.37)$, labelled D in the figure.

It relocates finally with rapid motion in the X and Y directions to $(-1.37, 98.10, 103.48)$, shown as E in the figure.

The molecule P_{20500} , labelled A in Figure 8, is at $(-9.18, 45.90, 104.04)$ initially. It moves relatively rapidly, primarily in the Y direction, to $(-14.07, 89.81, 79.32)$, labelled B in the figure. It then descends in a somewhat spiral fashion to its terminal point $(-25.74, 50.31, 52.15)$, labelled C in the figure.

The molecule P_{22500} , labelled A in Figure 9, is at $(24.48, 24.48, 104.04)$ initially. Its initial motion is rapid in Y direction to $(19.13, 93.83, 102.7)$, shown as B in the figure. It then descends to $(21.29, 78.43, 57.96)$, shown as C in the figure, and finally sidles its way down to $(2.74, 72.29, 46.76)$.

The molecule P_{23500} begins at $(15.30, 58.14, 97.92)$, shown as A in Figure 10. It moves rapidly in the Y direction to $(35.16, 99.32, 99.51)$, shown as B in the figure. From there it slides its way downward in an oscillatory fashion to its final point $(50.96, 95.27, 66.07)$, shown as C in the figure.

In each of the above examples, extensive motion results because the initial point is relatively close to the moving face. Molecular motion in the bottom of the cavity was far less extensive. Motion in the corners usually appeared to consist of random local oscillations.

Figure 11 shows a direct, two dimensional simulation of the flow in the YZ plane for wallspeed 25, $J = 25200$ and $\Delta t = 0.00008$ at $T = 7.04$. The initial data are those for the molecules in the YZ plane in the three dimensional example described above. The flow is analyzed using the very same parameters as those used to display Figure 5. Comparison of the results in Figure 5 and those in Figure 9 show that there is a distinct difference in the two dimensional and three dimensional simulations. The average speed of the molecules in Figure 9 is $4.3574 \text{ \AA/ps}$, while those in Figure 5 is $8.2368 \text{ \AA/ps}$. In addition, the molecular distributions, though similar, are different. The differences are due to the presence of forces in three dimensions which play no role in the two dimensional simulation [15].

Note that if one defines the Reynolds number Re by $Re = VB/\nu$ [5], in which V is the wall speed, B is the span, and ν is the average kinematic viscosity of water, then, for the example above, $V = 25 \text{ \AA/ps}$, $B = 104.04 \text{ \AA}$, and, at 15° C , $\nu = 113.12 \text{ \AA}^2/\text{ps}$ [16], so that $Re = 23.01$.

For our next example, set $V = 100$ ($Re = 92.04$), $\Delta t = 0.00004$, and $J = 14000$. Figures 12-16 show the vortex development in the YZ plane at the respective times $t = 2.90, 3.35, 4.02, 7.04, 10.07$. As in the first example, the velocities are reduced in the figures by $mv = 0.51$ for graphical clarity. Results using $J = 11200, 16800, 19600$, and 22400 yielded results entirely similar to those for $J = 14000$. The mean speed at 10.04 in Figure 16 is $10.56 \text{ \AA/ps}$. This result, when compared with the mean speed of $9.46 \text{ \AA/ps}$ for wallspeed $25 \text{ \AA/ps}$, indicates that an increase in wallspeed by a factor of four may not result in a proportionate increase in fluid speed throughout the cavity. This is probably due to the strong damping at the walls and due to the fact that much of the lower half of the cavity has still not been affected significantly by the motion of the upper wall. Indeed, in Figure 6 the lower half of the cavity has 747 molecules with a mean speed of $4.63 \text{ \AA/ps}$, while in Figure 16 the lower half of the cavity has 741 molecules with a mean speed of $4.69 \text{ \AA/ps}$.

In plotting Figures 12-16 for $V = 100$, the following rule of thumb was used. Since V is four times greater than, while Δt is half that for $V = 25$, we chose $J = (.25)(2)(25200) = 12600$. However, data had not been saved for this value of J , so we chose the next larger value, i.e., 14000, for which data was available. In this connection, note that if one chooses J too large, physically unrealistic results can follow for primary vortex motion. For example, if for $V = 100$ one chooses $J = 28000$, then the average speed at $t = 10.07$ for the velocity field is only 8.23 Å/ps, which is less than that for $V = 25$ at the same time.

Comparison of Figures 2-6 and 12-16 show the more rapid development of the primary vortex for $V = 100$. It should be observed, however, that the vortex in Figure 6 is at a relative steady state, whereas the vortex in Figure 16 is not.

Though individual molecular trajectories showed more motion than those displayed in Figures 7-10, the relatively low value of Re did not yield results of particular interest, like those which result in Taylor-Görtler vortices. For this reason, we concentrated attention on secondary vortices at $t = 10.07$.

Since secondary vortices have rotational speeds much smaller than primary vortices, it is necessary to use relatively large values of J to display these. Thus for $J = 56000$, Figure 17 shows the secondary vortex in the lower right corner, while for $J = 50000$ Figure 18 shows the secondary vortex in the lower left corner. That there are only two secondary vortices at $Re = 92.04$ is consistent with the experimental results in this range of low Reynolds numbers [14]. We were able to find only one secondary vortex for $V = 25$, and this was in the lower right corner.

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