Molecular Collision Frequency with a Dipole-Dipole Interaction

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Vast majority of previous dynamic cluster population simulations have treated cluster collisions as those of spheres without any interaction potential. Modelling can be improved on by studying the influence of an interaction potential on the collision frequency. We have constructed a program to solve trajectories of two interacting polar molecules. The program is based on the classical equations of motion and we have studied the collision frequency of two polar molecules by assuming the molecules to be spherical with dipole moments. In addition, we have studied the impacts of varying radius, mass and dipole moment on the collision frequency of the molecules. We have also applied the program to study the collision frequencies of certain larger clusters containing sulfuric acid and DMA.

We have used classical electrostatics to solve the force between the polar molecules. We have taken into account how the orientations of the dipole moments affect to this force and included in the influence of the interaction to the angular velocities.

The constructed program simulates two polar molecules or clusters and determines whether they collide with each other. The molecules have initial velocities and angular velocities which are drawn from Maxwell-Boltzmann distributions. Velocity Verlet algorithm (Scope, 1982) is used for both positions and rotations of molecules in order to solve the trajectories of the molecules. A collision is defined to occur if the distance between two molecules is smaller than the sum of the radii of the molecules. In Figure 1 there is an example from a simulation which ends to a collision.

The program was first tested by using the potential between an ion and a neutral molecule (Dugan, 1967) and we achieved a good correspondence with the theory.

We will report the collision frequency of sulfuric acid and DMA molecules and information how varying the radii, the masses or the dipole moments of these molecules affects to the collision frequency. In addition, we will study the collision frequencies of clusters that are listed in Table 1.

Simulated molecule or cluster pair
H_2SO_4 - H_2SO_4
H_2SO_4 - NH_3
$(H_2SO_4)(C_2H_7N)$ - $(H_2SO_4)(C_2H_7N)$
$(H_2SO_4)_4(C_2H_7N)_3$ - $(H_2SO_4)(C_2H_7N)$
$(H_2SO_4)(H_2O)_2$ - $(H_2SO_4)(H_2O)_2$

Table 1. The simulated molecules and clusters pairs.

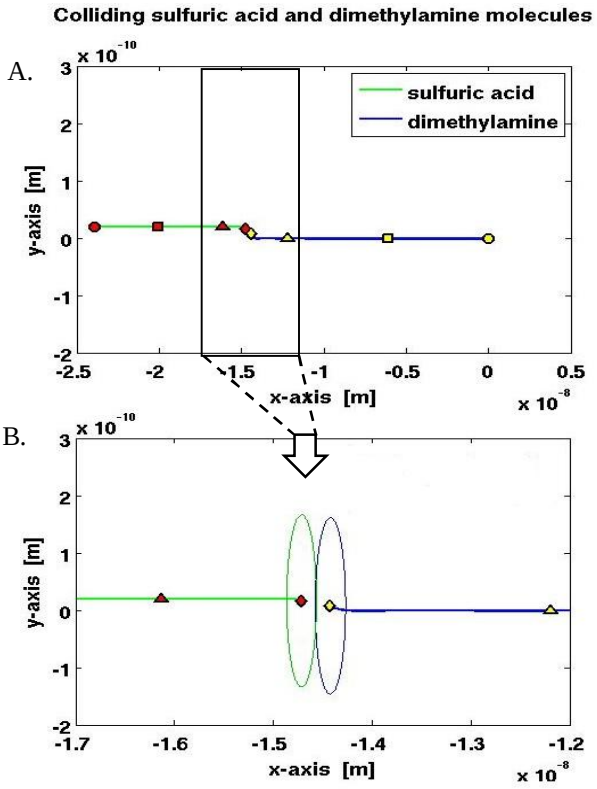

Figure 1. An example from a dipole-dipole simulation in which a collision does occur. The markers represents the positions of molecules at the specific moment of time. Circles representing the radii of the molecules at the moment of the collision are drawn in Panel B.

Scope, W.C., Andersen, H.C., Berens, P.H., and Wilson, K.R.: A computer simulation method for the calculation of equilibrium constants for the formation of physical clusters of molecules: Application to small water clusters, *The Journal of Chemical Physics*, **76**, 637 (1982); doi: 10.1063/1.442716

Dugan Jr, J.V., and Magee, J.L.: Capture Collision between Ions and Polar Molecules, *The Journal of Chemical Physics* 47, 3103 (1967); doi: 10.1063/1.1712359