Nanoscale Volumes’ Admixture Transfer In Relation To Molecules with Casimir Force: A Simulation of Interactions Involving Physical Characteristics’ Statistical Distributions

Firas sh. Fandi1, Sahira M. Yaseen2

Frissker1978@gmail.com1, Sahira.mahmood@gmail.com2

Abstract--The main aim of this study was to investigate admixture molecular systems relative to their statistical properties. The admixtures under investigation were those placed in Nanoscale volumes such as parallelepiped and cube settings having wall impermeable surfaces. Free molecule interactions were simulated in admixtures relative to wall surface molecules. In turn, the interactions were modeled based on atomic structure grids. Also, SiO2 was used as a material and its use was informed by the ability to account for important quantum effects’ manifestations; Casimir force in this case. It is also notable that a random distribution function for surface heights was used to model the roughness of the target surface. Some of the parameters to which the results were applied for estimation included polyatomic molecules’ dihedral angle length deviations, valence, and chemical bond lengths. From the results, it was evident that the proposed model can determine a system’s stable configuration properties, upon which practical problems could be solved relative to physical limitation conditions of Nanoscale devices – especially in highly dispersed systems’ admixture filtration. With the impact of Casimir force on admixture volumes examined and multi-component admixture membranes or plates’ radial distribution function computed, results demonstrated distributions of lengths relative to their associated equilibrium values.

Keywords—admixtures, Nanoscale, equilibrium

1. Introduction
In nanoscale dynamic systems, molecular structure modeling forms one of the most relevant studies [1, 2]. This trend has been documented especially for scenarios involving molecular structures through which materials with improved or new characteristics are produced [3, 4]. Another relevant area involves the determination of equilibrium states [5], as well as the definition of deviation intervals [6], which play a crucial role in areas such as biotechnology and medicine, as they affect outcomes regarding the gene modification or viruses and proteins [7, 8]. It is also noted that the production of nanoscale systems that are resistant to the influence of the environment and also highly efficient is of importance [9], especially in applications of technical disciplines and natural science [10]. Some of the problems that have been observed to face molecular structure modeling include calculating the distribution of crucial parameters, the comparative analysis of models, and aspects such as agglomerates, admixtures, and clusters in technical systems [4-6]. Given that mathematical frameworks with high parallelization calculations have been employed, intensive computer work is worth conducting [5]. For such problems, previous studies avow that the development and solutions have been achieved through numerical simulation techniques [4-7]. However, situations where real systems’ distances between surfaces are less than 10 nanometers have posed technical difficulties [1, 5]. The eventuality is that there has been a growing need to consider strong interaction and quantum effect contributions. In this study, the use of Casimir force was considered. The study examined the impact that a system’s statistical properties’ volumes that are produced are likely to pose. Specifically, the study examined how chemical bonds might have equilibrium values distributed in polyatomic molecules. The eventuality is that a model that focuses on interaction potentials such as CHARMM and AMBER was proposed.
2. Methodology – The Mathematical Model

In the proposed model Casimir force played a crucial role. Whereas it is characterized by a quantum nature, the force could also be established in terms of the interaction energy potential, hence the classical approximation. For the admixture molecules, they were set randomly in the grid of the virtual inner volume before being distributed uniformly. In so doing, the net potential energy’s minimum was achieved initially. The mathematical optimization was developed in the form:

\[
\frac{\partial^2}{\partial t^2} \mathbf{r}_i = -\nabla \left[ \sum_{\text{pairs}} U_b + \sum_{\text{triples}} U_a + \sum_{\text{quadruples}} U_d + \sum_{i<j} \left( U_{ij}^{LJ} + U_{ij}^{col} + U_{ij}^{c} \right) + \sum_{\text{wall}} U_{\omega} \right]
\]

The experimental initial conditions were in the form:

\[
\mathbf{r}_i(0) = \mathbf{r}^0_i; \\
\frac{\partial}{\partial t} \mathbf{r}_i(0) = \dot{\mathbf{r}}^0_i;
\]

Figure 1: The selected Casimir energy interaction process for an atom-atom framework
Another notable path involved the interaction between the modeled volume’s inner walls and Casimir force. To ensure that the proposed model utilized Casimir force, a well-known expression for the force was integrated. The integrated expression was that which depended on the interacting area and the distance of the wall-admixtures or corresponding atoms. It is also notable that the box surfaces were modeled to assume the form of molecular structures. The eventuality is that same-type atom-atom interactions were used to calculate the parameters for the respective atoms in the admixtures’ molecules. Indeed, one of the central assumptions that were made was that there were constant and average values for the selected neighbor atoms covering the admixture atom projections in relation to the selected or target wall surfaces. With four neighbor atoms on the target, the shortest distances to the admixtures’ interacting atoms were determined by:

\[ U_c(r_{ij}) = -\frac{1}{4} \sum_{\text{neighbors}} \frac{\pi^2 \hbar c}{720r_{ij}^3} \]

Additional statistical analyses were conducted via the computation of the distributions of moderating factors or parameters such as the dihedral angles displacements, valence, and bond lengths. For the admixtures, these analyses were conducted in radial distribution and polyatomic forms via the equation:

\[ g(r) = \frac{V}{4\pi r^2} \left\langle \sum_{i=0}^{N-1} \frac{n(r_i)}{\Delta r} \right\rangle \]

Regarding the computational experiments, it remains notable that two forms of simulated geometries were modeled. These geometries were those involving comparable inner volumes. Specifically, the selected geometries constituted a parallelepiped with upper and lower bases and a cub of 10 nanometers. With the volumes selected, the same amounts of admixtures were used to fill them. The selected admixtures had 25 molecules of the respective forms of substances. The substances entailed ethanol, water, oxygen, hydrogen, and nitrogen. Given the lower and upper bases of the boxes, two forms of reflections were simulated in terms of specular reflections and the diffuse model. The figure below summarizes the computational experimental setup.
3. Results, Analysis, and Discussion

In blocks of potential energies calculations, numerical methods and a mathematical model were implemented. To determine or predict the potential impact of Casimir force on parameter interactions, non-periodic boundary conditions were modeled through the development of the original package. Imperative to note is that the proposed model did not rely on the truncation of the lengths of potential functions, a trend that was adopted in situations where distances exceeded three diameters of the selected atom-atom collisions.

As mentioned earlier, the motivation of the study was to give insight into how data simulation could aid in unstable state predictions, as well as material deformations and overheating on certain mechanisms’ walls with parallel surfaces. In this study, the proposed model was capable of supporting the design of mechanisms with membranes, solar cells, and filter elements in which there is a possibility of the occurrence of nonlinear effects relative to surface reflectivity and the nature of the material. For ethanol and water molecules, the resultant distribution was observed to have a high density of values closer to the equilibrium state. However, the right of the equilibrium value for these molecules saw a gentle spread and a small subset of values reported. In relation to the case of the parallelepiped arrangement, there was normal distribution, which did not change. Another crucial observation arising from the proposed framework’s implementation was that as the number of admixtures increased, the highest concentration
was achieved behind the volumes’ corners. It was evident further that the Casimir force poses a significant impact on equilibrium value distribution in relation to chemical and physical characteristics of the admixtures. These results or inferences were informed by length deviations when passing through air purification systems, during the adsorption of harmful substances, and membrane behaviors on infiltration devices.

4. Conclusion

In summary, the Casimir force was observed to have a significant effect on the mean value distributions for the case of dihedral angles deviations, valence, and covalent bond lengths; with polyatomic molecules on the focus. For the case of cubic volumes, the latter impact of the force was informed by changes in the type of distribution, as well as the displacement of the distribution center. Regarding the case of parallelepiped, the inference regarding the significant posed by the Casimir force was informed by a situation in which most of the lengths values were observed to concentrate around the equilibrium values. Another notable trend that was observed from the modeling was that given the surfaces of the structure of volume, the high density of the atoms and strong intermolecular electrostatic interactions cause a significant increase in the relaxation time of valence angles and the covalent bonds, upon which non-equilibrium processes accumulate. For the case of the parallelepiped, there was an increase in the average deviations of values’ dispersion relative to the angles of chemical bonds and the equilibrium lengths.

5. References

[1]. L. A. Uvarova and S. S. Babarin, “Themovement of molecules and nanoparticles in potential field with the Casimir force in nano volumes with different optical boundaries,” Physica Scripta, vol. 2014, 2014.

[2]. B. Hess, K. Carsten, D. van der Spoel, and E. Lindahl, “GROMACS 4: algorithms for highly efficient, load-balanced, and scalable molecular simulation,” Journal of Chemical Theory and Computation, vol. 4, no. 3, pp. 435–447, 2008.

[3]. H. B. G. Casimir, “Proceedings of the Koninklijke [18] R. Sadus, Molecular Simulation of Fluids: Theory, Algorithms and Object-Orientation, 2002.

[4]. S. S. Babarin and L. A. A. Uvarova, “Mathematical modeling of non-equilibrium processes in nano volume the happening as the Casimir’s force acting,” Dynamics of Heterogeneous Systems, vol. 29, no. 1, p. 60, 2007

[5]. M. Bordag, U. Mohideen, and V. Mostepanenko, “New developments in the Casimir effect,” Physics Reports, vol. 353, no. 1-3, pp. 1–205, 2001.

[6]. L. Gross, F. Mohn, N. Moll, P. Liljeroth, and G. Meyer, “The chemical structure of a molecule resolved by atomic force microscopy,” Science, vol. 325, no. 5944, pp. 1110–1114, 2009.

[7]. A. A. Panteleev, B. E. Ryabxhikov, O. V. Horuzhiy, S. L. Gromov, and A. P. Sidorov, Technology of membrane separation in industrial water treatment - M.: DeLi plus, 2012.

[8]. D. R. Lide, CRC Handbook of Chemistry and Physics, Taylor & Francis, New York, NY, USA, 90th edition, 2009.

[9]. Y. Chiang and P. Wu, “Adsorption equilibrium of sulfur hexafluoride on multi-walled carbon nanotubes,” Journal of Hazardous Materials, vol. 178, no. 1-3, pp. 729–738, 2010

[10]. P. D. Gujrati, “Loss of temporal homogeneity and symmetry in statistical systems: deterministic versus stochastic dynamics,” Symmetry, vol. 2, no. 3, pp. 1201–1249, 2010.