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Review Article

"Diffusion" and The Basic Nature of Intermolecular Attraction Forces

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Abstract

Here in this paper, we show that the primary reason for this diffusion is the intermolecular attraction forces due to Newtonian gravitational attraction forces acting in a combined way which are the vectorial sum of all the attraction forces acting on molecules as defined as SITA forces Multi Molecule Theory. Some pairs of molecules hit each other, bounce like rubber balls, and diffuse because of these SITA forces. Here some of the molecules are going to higher distances from the hitting centers. Earlier we formulated and showed the three states of matter similarly. Here we took a Nano-drop-let of contaminated water as a container. We are calculating inter-molecular attraction forces between molecules and finding the movements of molecules due to the attraction by all the other molecules at the molecular level.

Keywords: Diffusion; Newtonian Gravitation; Hydrodynamics; Molecular Data; Multi Molecular Theory; SITA Simulations; Dynamic Universe Model

Introduction

How to detect these inter molecular hits? For that, we used Visual Basic for Excel and developed macros to find these hits. This development took almost 18 months.

Thus, we detected intermolecular hits happened in an iteration. We collected addresses of inter-molecular hits in a chosen area in the spreadsheet. The overall shape of area where hits are stored, is changing with inter molecular distances. We experimented by changing all the inter molecular distances proportionally without changing the relative positions of molecules with each other and captured the screen-shots. That is how the first author showed the three states of matter happen in the previous paper. See paper by first author in April 2022. This SITA calculation method can be applied to any chemical in liquid or gaseous state.

This present paper is the next step. After we detected above mentioned hits, we observed some pairs of molecules travelling longer distances from the center of the used molecules set. This is 'Diffusion'. Clearly this is happening after the hit, so this this diffusion is not bulk flow.

It may please be noted, here we were not considering the earth's gravitation in the present set of calculations. This is also a fundamental result. In our quest to find the basic nature the intermolecular attraction forces, we worked out this third paper. There will be some more results to answer some further questions like Brownian motion and Navier-stokes equations etc.

Intermolecular attraction forces

- We know the Van Der Waals Forces (London dispersion forces), which can be observed in all types of molecules

(1937). Tadmor [1] gave an interesting application of Van der Waals forces in various geometries. It should be noted Van der Waals forces need induced Dipoles. We will discuss about this in 3.1.

- In this paper, we are working on a new type of intermolecular force that is applicable for all types and species of molecules and which will NOT involve any type of Intermolecular Ion or DIPOLE attractions. This inter molecular force is purely Newtonian Gravitation based and depends on the collective vectorial sum of attraction forces of mass of molecules only.
- Let's go into details of our work….

SSMMT formation

Dynamic Universe Model's SITA simulation n-body solution software is the mother of all these developments. We changed physical values original astronomical masses and distances values of SITA software, with molecular masses and inter molecular distances values of water and its contaminations. Original SITA software does not have the provision for detecting HITs. This new software is now supplemented with newly developed software for finding inter molecular HITs.

Not enough force between any single pair of Molecules is created just by Newtonian Gravitation as the force of attraction. But the collective 3D vectoral sum of these forces of all surrounding Multiple molecules is sufficient. This was what exactly done in SSMMT.

Here we use Savitri Subbarao Multi Molecule Theory (We call this SSMMT) which are SITA equations of Dynamic Universe Model. We use them for finding inter molecular forces, inter molecular hits which gave results like explaining the states of matter, and which will lead into Brownian motions, coefficient of diffusion, Navier-Stokes equations etc. We don't use the age old 'Single Molecule theory'.

We calculate the resulting 3D force vector on a single molecule due to all the other molecules in our NANO droplet. This calculation procedure is repeated for all the molecules in the droplet with the help of SSMMT.

History

In 1959, Alder and Wainwright[4] used an IBM 704 computer to simulate perfectly elastic collisions between hard spheres. In his paper "Correlations in the Motion of Atoms in Liquid Argon" in 1964, Rehman A., said "The pair-correlation function and the constant of self-diffusion are found to agree well with experiment; the latter is 15% lower than the experimental value.

Assembly of molecules in test tubes usually hinder the behaviour of single molecules. The ensemble averages out the behaviour of single molecules. Daniel Riveline's [2] work on, 'Single molecule': theory and experiments showed this. SSMMT approach solves this problem.

We found many references of earlier physicists worked and experimented on values of 'force of attraction between molecules.' Even some contributors that calculated the approximate value of this force. But NONE of the earlier physicists worked directly on the BASIC NATURE of this 'force of attraction between molecules'.

Mathematical background for multi molecule theory

Let's take an example of H2O, this example can be any chemical or Eutectic solution like steel….

Let us assume a set of N mutually gravitating point masses viz molecules with some finite radii 'r'. They are moving due to Newtonian Gravitation, in a Nano drop of a colloid. Let this colloid be a mix of water molecules, Individual proteins, polymers of living matter such as DNA, RNA, actin or microtubules, molecular motors etc. Let these molecules don't react chemically with each other. So, all these molecules behave like perfectly elastic rubber balls bouncing. This set of molecules will have different sizes and different masses depending on molecular weight. These Nano-Particles move due to mutual gravitation attraction forces between individual molecules. Let's take total number of molecules to be 133, in a Micro-cubical having invisible and perfectly elastic walls. Use 3D Cartesian coordinates with some appropriate center of its axes in a beaker of the colloid to go further into the calculations of SSMMT.

Any molecule hitting the boundary will bounce back in accordance with Newtons laws. We will use nano distances and pico-second times as suitable. There will be bumping and collisions between some pairs of particles, and each nano particle will move and trace their path back after the elastic collision between the two. We can detect collisions by SSMMT software by two bumping particles when the center-to-center distance is less than or equal to the sum of two molecular radii of these Nano-spheres.

In this paper we will not consider gravitational repulsion at very low distances, only the bumping will happen at that distance.

Similarly, we will introduce the Viscosity forces in another forthcoming paper.

Assume a set of N mutually gravitating Nano(bio)-particles/ point masses under Newtonian Gravitation with some finite radii r_i These radii we will use for the calculation of bumping or collision in the SSMMT software.

Let the α^{th} point mass has mass m_α, and is in position x_α. In addition to the mutual gravitational force, there exists an external φ_{ext}, due to other molecules which also influence the total force F_α acting on the point -mass α. In this case, the φ_{ext} is not a constant universal Gravitational field but it is the total vectorial sum of fields at x_α due to all the external to its system bodies and with that configuration at that moment of time.

Total Mass of system =: $M = \sum_{\alpha=1}^{N} m_\alpha$ ---------- (1)

Total force on the point massα is Fα, Let $F_{\alpha\beta}$ is the gravitational force on the α^{th}point mass due to β^{th}point mass.

$$F_\alpha = \sum_{\substack{\alpha=1 \\ \alpha\neq\beta}}^{N} F_{\alpha\beta} - m_\alpha \nabla_\alpha \Phi_{ext}(\alpha) \qquad \text{---------- (2)}$$

The full set of equations and full derivation is available in the paper by First Author (2018). We are just giving these equations 1 to 3 here.

Total AGGREGATE Equations :(Aggregate consists of many Ensembles and systems)

Assuming these forces are conservative, we can find the resultant force by adding separate forces vectorially from equations.

$$\Phi_{ext}(\alpha) = -\sum_{\substack{\beta=1 \\ \alpha\neq\beta}}^{N^\gamma} \frac{Gm_\beta^\gamma}{\left|x^{\gamma\beta} - x^{\gamma\alpha}\right|} - \sum_{\substack{\beta=1 \\ \alpha\neq\beta}}^{N^{\delta\gamma}} \frac{Gm_\beta^{\delta\gamma}}{\left|x^{\delta\gamma\beta} - x^{\delta\gamma\alpha}\right|} \qquad \text{---------- (3)}$$

Dynamic Universe Model never condenses to General relativity on any condition. It uses a Linear tensor mathematics based on Newtonian physics are used here. All the math-derivations and the SITA (Simulation of inter-intra taught ness and attraction forces) an Lotus/Excel based software was developed about 40 years back on two floppy based computers of that time. SITA is singularity-free and dynamically stable. Those details are explained in the three books published by the first author Gupta SNP [2010, 2011, 2011]. Some of the other papers published by the first author are available at refs. [Published in years 2014,2015, 2016, 2017 2018, 2019 2020, 2021 2022] [3-23].

We applied above theory and developed an Excel sheet. See the data availability statement for the fully functional Excel sheet referenced just before the References in this paper.

Diffusion

The following figures show diffusion in water. Here larger molecules are being thrown away, the scales of the graph are increasing.

Now see inside the small cluster also if the molecules inside are moving.

Graph observations

- Relative positions in Graphs looking the similar, center is moving, but scales are different and changing from Graph to Graph, which indicates molecules are expanding.
- 10e5 molecules were taken in place of a single molecule, assuming a tine water droplet will have 10e25 molecules in it. This assumption will give calculatable and graphable movements in the molecule positions in Excel.

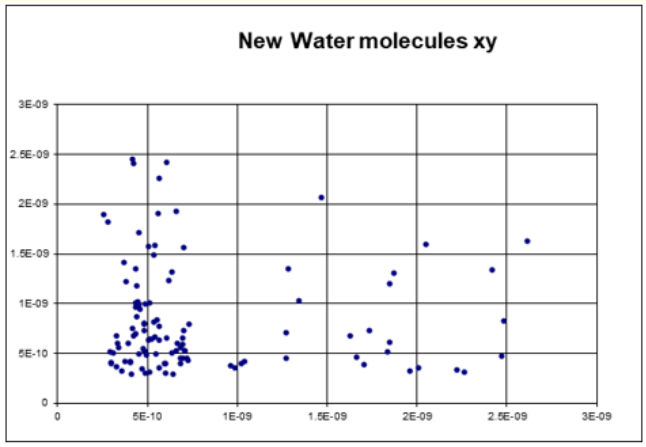

Figure 1: Output of 1st iteration with 100000 times mass of molecules in the simulation. This Figure shows xy projections graph. Figure 2 shows positions of higher atomic weight molecules of the same.

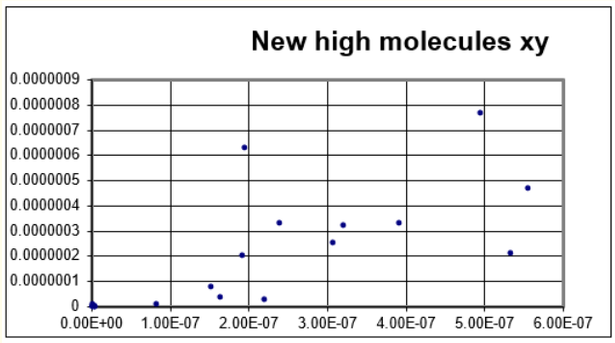

Figure 2: Output of 1st iteration with 100000 times mass of molecules in the simulation. Figure 1. shows xy projections graph. Figure 2. Shows positions of higher atomic weight molecules.

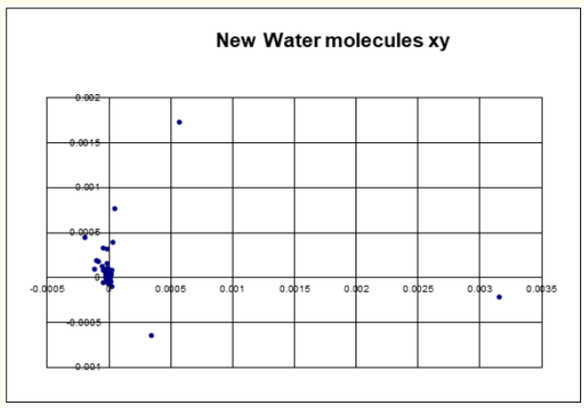

Figure 3: Output of 2nd iteration with 100000 times mass of molecules in the simulation. Figure 3 shows xy projections graph. Figure 4 shows positions of higher atomic weight molecules in all these graphs. Observe the new positions in these graphs how much different from earlier graph.

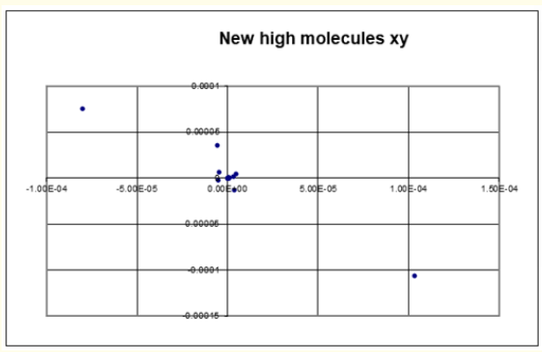

Figure 4: Output of 2nd iteration with 100000 times mass of molecules in the simulation. Figure 3 shows xy projections graph. Figure 4 shows positions of higher atomic weight molecules in all these graphs. Observe the new positions in these graphs how much different from earlier graph.

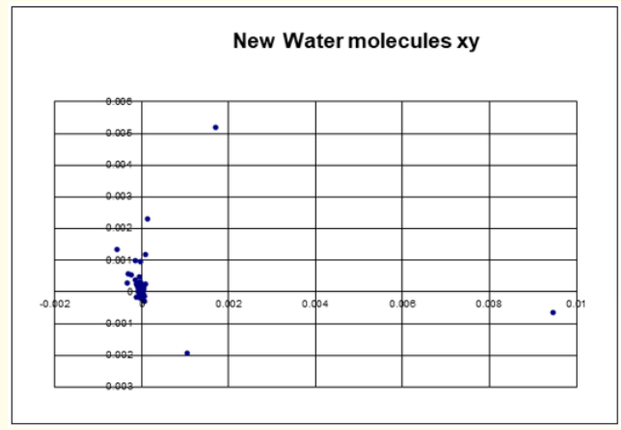

Figure 5: Output of 3rd iteration with 100000 times mass of molecules in the simulation. Observe the new positions in these graphs how much different from earlier graph. The distance travelled by two molecules from the center. Diffusion started to be visible here.

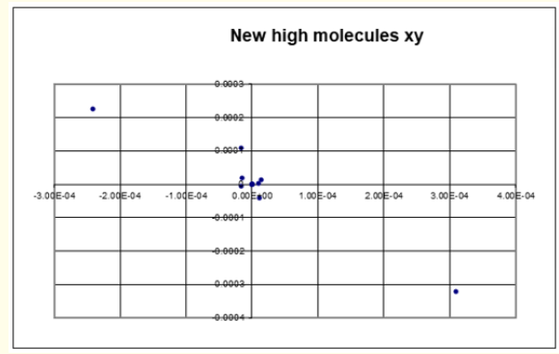

Figure 6: Output of 3rd iteration with 100000 times mass of molecules in the simulation. Observe the new positions in these graphs how much different from earlier graph. The distance travelled by two molecules from the center. Diffusion started to be visible here.

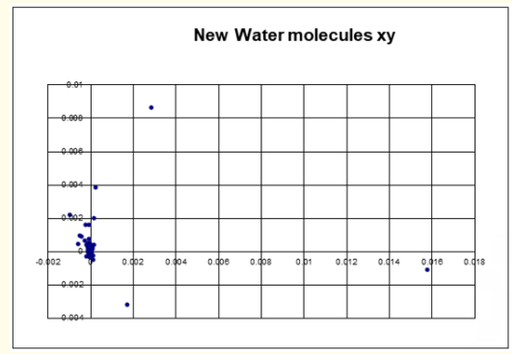

Figure 7: Output of 4th iteration of the simulation. Observe the new positions in these graphs how much different from earlier graph. The distance travelled by 4 molecules from the center in Figure 7 graph and 3 in Figure 8. Diffusion started to be more visible here.

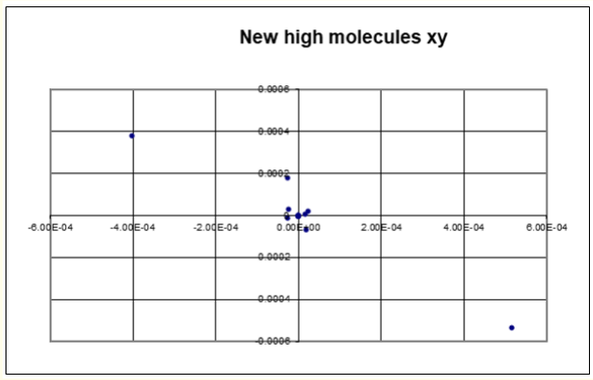

Figure 8: Output of 4th iteration of the simulation. Observe the new positions in these graphs how much different from earlier graph. The distance travelled by 4 molecules from the center in Figure 7 graph and 3 in Figure 8 diffusion started to be more visible here.

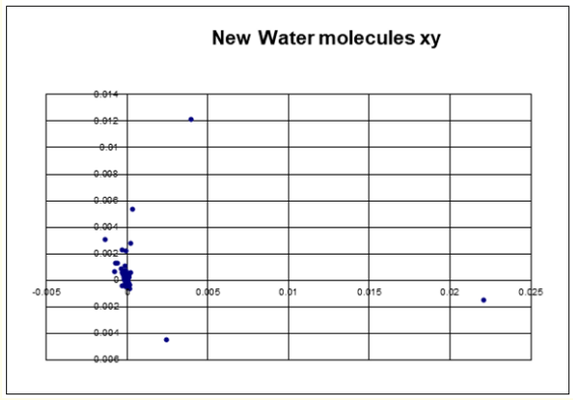

Figure 9: Output of 5th iteration of the simulation. Here the Center also moved. The distance travelled by 5 molecules from the center in Figure 9 graph and 4 in Figure 10. Diffusion started to be more visible here.

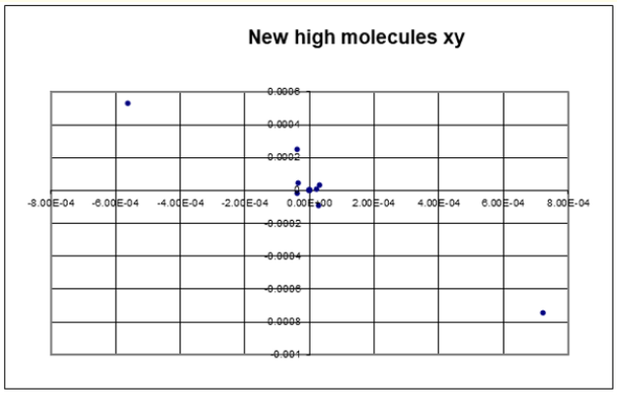

Figure 10: Output of 5th iteration of the simulation. Here the Center also moved. The distance travelled by 5 molecules from the center in Figure 9 graph and 4 in Figure 10 diffusion started to be more visible here.

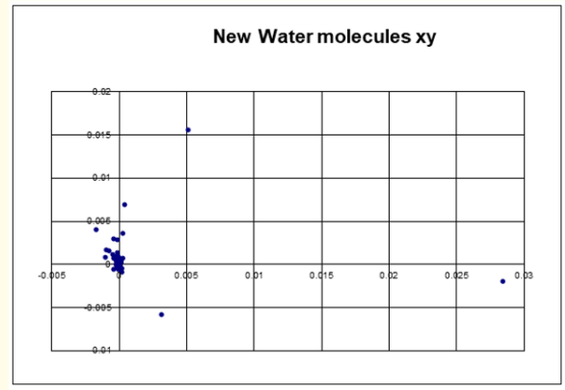

Figure 11: All Molecules: output of 6th iteration of the simulation. Here the Change in Scales can be seen, Center also moved and Graph widened. Center concentration of our molecules diffused.

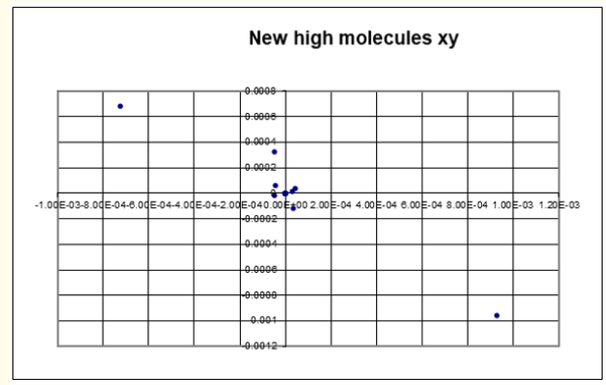

Figure 12: Heavy Molecules: Output of 6th iteration of the simulation. Here the Change in Scales can be seen, Center also moved and Graph widened. Center concentration of our molecules diffused.

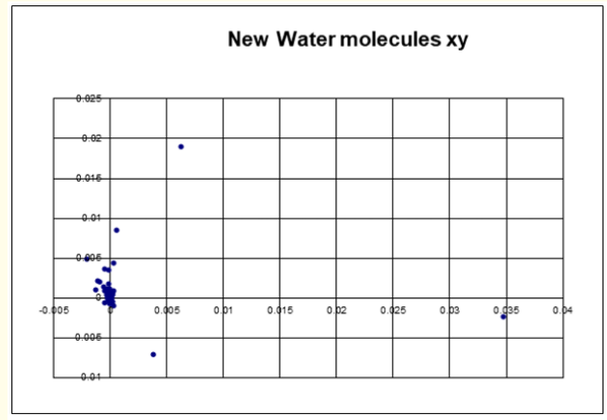

Figure 13: All molecules: Output of 7th iteration of the simulation. Here the Change in Scales can be seen, Center also moved and Graph widened. Center concentration of our molecules diffused.

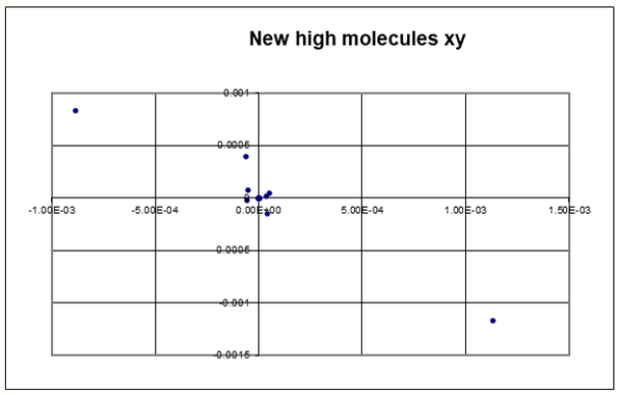

Figure 14: Heavy Molecules: Output of 7th iteration of the simulation. Here the Change in Scales can be seen, Center also moved and Graph widened. Center concentration of our molecules diffused.

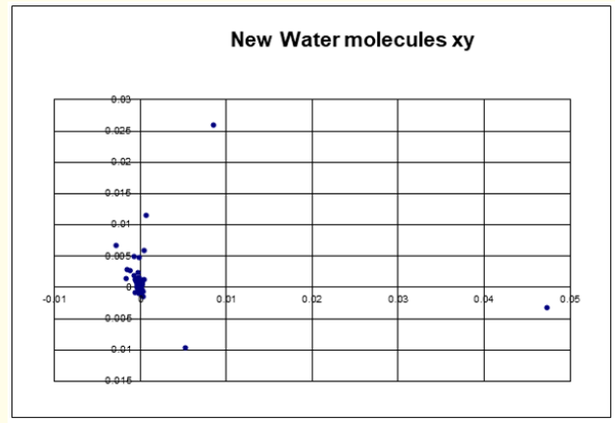

Figure 17: All Molecules: Output of 8th iteration of the simulation. Here the enter is moving. Center concentration of our molecules diffused.

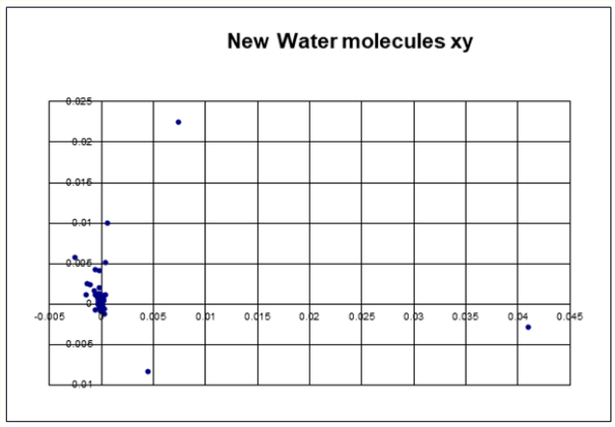

Figure 15: All Molecules: Output of 8th iteration of the simulation. Here the Graph widened. Center concentration of our molecules diffused.

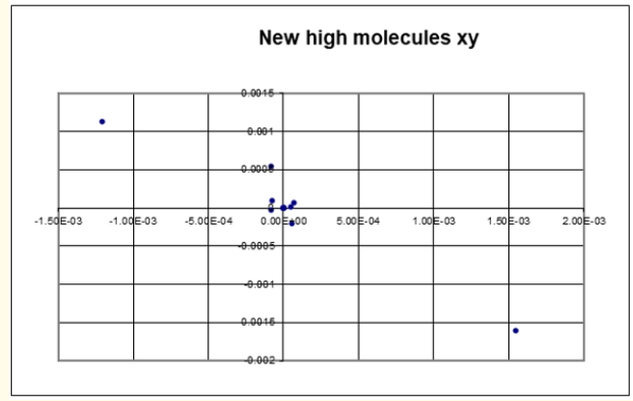

Figure 18: Heavy Molecules Output of 8th iteration of the simulation. Here the enter is moving. Center concentration of our molecules diffused.

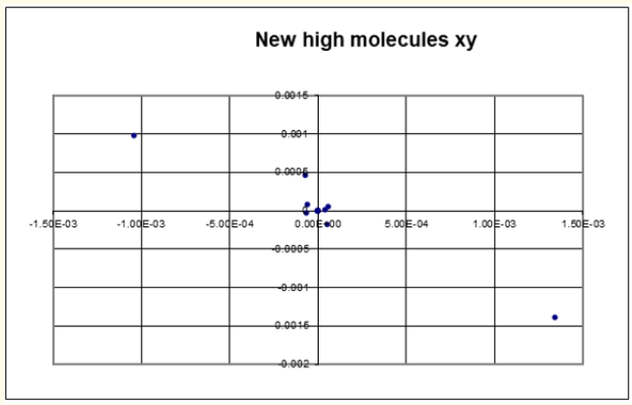

Figure 16: Heavy Molecules: Output of 8th iteration of the simulation. Here the Graph widened. Center concentration of our molecules diffused.

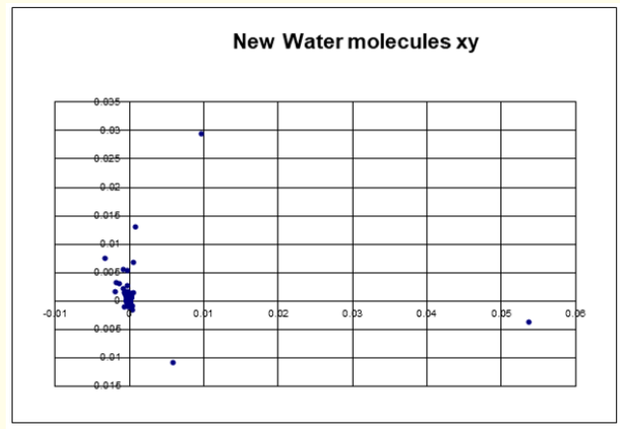

Figure 19: All molecules: Output of 8th iteration of the simulation. Here the enter is moving. Center concentration of our molecules is more diffused.

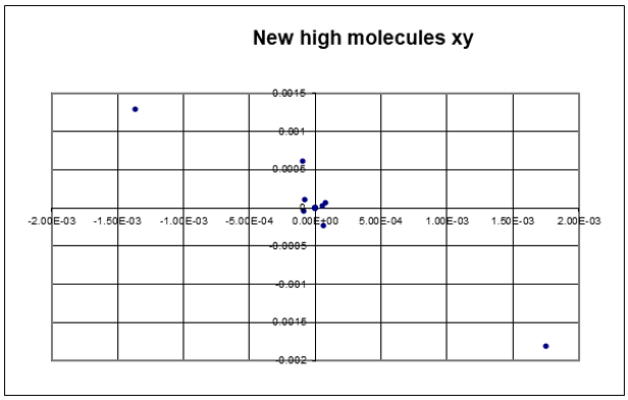

Figure 20: Heavy Molecules: Output of 8th iteration of the simulation. Here the enter is moving. Center concentration of our molecules is more diffused.

Further work will be leading to Brownian Motion. We have to contain these molecules in a box of fixed size and fixed coordinates. And allow these molecules to bounce with each other and with boundaries. Check the trajectories, that will be Brownian motion.

We already developed the Hits to all the 6 sides of variable size box with maximum and minimum coordinates and inter molecular hits.

Now we have to develop a way to analyse these hits and process them to further visualize the trajectories after all these hits.

[SSMMT - Multi molecule theory] vs [Sita Simulations of Dynamic universe model]

Basically in SSMMT and Sita Simulations use the same Mathematical framework. But we use the molecular masses and intermolecular distances instead of Astronomical distances and masses in SSMMT.

Discussion on SITA Simulations

SITA simulations solved many presently unsolved problems in Physics …

Nobody attempted to find the basic nature of intermolecular attraction forces. SITA simulations find that Newtonian Gravitation is necessary, appropriate, and sufficient for explaining the basic nature of intermolecular attraction forces between H2O molecules as defined by Multi Molecule theory. We already know SSMMT uses the collective gravitational attraction of all the molecules on any single molecule in the collection of molecules.

- Prediction of a large number of Blue-shifted Galaxies (>5) at the Universe Level.
- Missing mass due to Star circular velocities and Galaxy disk formation at Galaxy level,
- Pioneer anomaly at the Solar system level,
- For conversion of Energy to Matter at the Energy level.
- SSMMT Simulations: We used SSMMT Simulations for finding the Combined Vector Force using Newtonian Gravitation as Binding Force Between H2O Molecules for explaining the Basic Nature of Intermolecular Attraction Forces and gave the example of H2O to explain the formation of Three States of Water using SSMMT at Nanoparticle level.

We have various results like the experimental value of Inter Molecular attractive forces is Near to Newtonian gravitation and differences are explained by SITA simulations.

There are many applications of SITA simulation, like energy formation, various Element creation, for all papers on SSMMT and other papers and books please see our webpage in References.

Now we derived Diffusion in this paper with the same SITA framework.

Conclusion

Diffusion can also be explained by SSMMT.

This result provides another support for our original proposition, that the inter molecular forces are nothing but they are the 'sum' of Vector Forces using Newtonian Gravitation attraction as Binding Force Between Molecules or in other words.

SITA forces. Here in this paper, in other words, we used these SITA forces for explaining the Basic Nature of Inter Molecular Attraction Forces.

Earlier researchers found the value of attraction forces but I could not get any work showing the basic nature or reason of attraction of Inter molecular attraction. Another thing which was

well discussed in the scientific world is "Assembly of molecules in test tubes usually hinder the behaviour of single molecules. The ensemble averages out the behaviour of single molecules." Now with the help of this SSMMT we don't have to go for elaborate methods to Isolate single molecule, to do a variety of EXPERIMENTS with SIMPLER and CHEAPER LAB equipment.

Acknowledgements

I thank Mother Vak for the continuous guidance and encouragement for solving these totally unknown situations and helping me pass through all the hurdles to attain the victory of solving this problem.

Full EXCEL file and Data Availability

Satyavarapu Naga Parameshwara Gupta. (2021). We uploaded a file named 'Vak REF DF 1 hits in 8 col and scattered hits.XLS. in Zenodo. with a doi: https://doi.org/10.5281/zenodo.5569547.

Please download the file above. This file can be used for States of matter and for diffusion.

Additionally, the First author can be contacted for any data or quarry.

Bibliography

1. Tadmor R. "The London-van der Waals interaction energy between objects of various geometries". *Journal of Physics: Condensed Matter* 13.9 (2001): L195-L202.

2. Daniel Riveline. "Single molecule': theory and experiments, an introduction From Nanophysics for Health". *Journal of Nanobiotechnology*, Mittelwhir, France (2013): 5-9. November 2012 Riveline Journal of Nanobiotechnology 11 (2013).

3. Alder B J and Wainwright T E. "Studies in Molecular Dynamics. I. General Method". *The Journal of Chemical Physics* 31.2 (1959): 459-466.

4. Garrett, Reginald H.; Grisham, Charles M. "Biochemistry (6th ed.)". University of Virginia (2016): 12-13.

5. Gupta SNP. "Basic Nature of Three States of Water Explained by "Multi Molecule Theory"". A*cta Scientific Medical Sciences* 6.4 (2022).

6. GUPTA SNP. "Dynamic Universe Model: A singularity-free N-body problem solution". VDM Publications, Saarbrucken, Germany (2010).

7. Gupta SNP. ""Multi Molecule Theory" with Gravitation as Binding Force between Molecules Can Explain Brownian Motion-After Seeing Final Positive Results of SSMMT Simulation". *Journal of Molecular Sciences* 40.2 (2020).

8. https://vaksdynamicuniversemodel.blogspot.com/

9. Gupta SNP. SCIFED Journal of Nuclear Science. "Energy to Mass conversion in Dynamic Universe Model". 2 (2018): 2.

10. Gupta SNP. "Dynamic Universe Model: SITA software simplified". VDM Publications, Saarbrucken, Germany (2011)

11. Gupta SNP. "Basic Nature of Three States of Water Explained by "Multi Molecule Theory"". *Acta Scientific Medical Sciences* 6.4 (2022): 119-129.

12. Gupta SNP. "Dynamic Universe Model: SITA singularity free software". VDM Publications, Saarbrucken, Germany (2011).

13. Hamaker H C. *Physica* 4.10 (1937): 1058-1072.

14. https://en.wikipedia.org/w/index.php?title=Van_der_Waals_force&oldid=958850259

15. Israelachvili J. Intermolecular and Surface Forces. Academic Press (1985-2004).

16. Lipkowitz Kenny B and Cundari Thomas R. Reviews in Computational Chemistry. 26. John Wiley and Sons. pp. 39-90.

17. London F. *Transactions of the Faraday Society* 33 (1937): 8-26.

18. Meglio A., *et al*. "Single DNA/protein studies with magnetic traps". *Current Opinion in Structural Biology* 19.5 (2009): 615-622.

19. Parsegian VA. van der Waals Forces: A Handbook for Biologists, Chemists, Engineers, and Physicists. Cambridge University Press (2006).

20. Purcell C. "Life at low Reynolds number". *American Journal of Physics* 45 (1977): 3-11.

21. Schuler B and Eaton WA. "Protein folding studied by single-molecule FRET". *Current Opinion in Structural Biology* 18.1 (2008): 16-26.

22. Rahman A. "Correlations in the Motion of Atoms in Liquid Argon". *Physical Review* 136.2A (1964): A405–A411.

23. Tschumper Gregory S. "Reliable Electronic Structure Computations for Weak Noncovalent Interactions in Clusters" (2008).