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Review Article

Basic Nature of Three States of Water Explained by "Multi Molecule Theory"

Satyavarapu Naga Parameswara Gupta*

Retired Assistant General Manager, Bhilai Steel Plant, Bhilai, India

***Corresponding Author:** Satyavarapu Naga Parameswara Gupta, Retired Assistant General Manager, Bhilai Steel Plant, Bhilai, India.

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Abstract

This is a vital result. We know the three main states of H_2O, viz., ice, water and vapour. What is the reason for this change of state? What is the inherrant nature the inter molecular attraction forces? These questions were not thought off earlier. On what factor that makes H_2O to change its state. Of course, temperature is the common answer. We plunged into a more fundamental aspect i.e., inter molecular attraction forces and intermolecular distances. We took a distance factor (DF) = 1 which represents inter molecular distances in a drop of contaminated water. And keeping the original molecular structure same changed all the inter molecular distances proportionally with different values of DFs… We wrote macros in Visual Basic for Excel to find the inter molecular hits that would happen for that DF from the excel sheet where all the calculations were done. We plotted addresses of colliding molecules in a designated area in the worksheet. We took screen shots of that area for that value of DF value and shown these plots Inter Molecular Hits in this paper. We observe that number of inter molecule hits is decreasing from all the pairs hitting each other to no hitting pair depending on inter molecular distances. We can visualize very clearly for DF 0.02 to 0.08 the state will be ice, for DF 9 to 300 the state will be water and for DF 5000 to 10000 the state will be vapour. There are many MIXED intermediate states.

Keywords: Gravitation; Acceleration of Particles; Dynamic Universe Model; Molecular Processes; Molecular Data; Multi Molecular Theory

Introduction

This paper is a further application of theory presented and published in Journal of Molecular sciences by us (2020) using this Savitri Subbarao Multi Molecule Theory (We call this SSMMT). We can use these equations not only for inter molecular forces, inter molecular hits due to Brownian motions in this paper, but also we will be using them to develop some equations for coefficient of diffusion etc.

We took the same contaminated water droplet in space in a distant place where gravitation effects of other bodies of Universe can be neglected. Here we will calculate the resulting force vector due to Newtonian gravitation on every single molecule due to all the other molecules in the droplet. We must mention that just "Newtonian Gravitation" as the force of attraction is NOT sufficient to give enough force between any single pair of Molecules. We enhanced the masses of molecules with a factor 10^{10} (assuming that there will be that many molecules are in that line acting to develop attraction force) so that the forces will come into calculatable range of Excel we are using here with the help of SSMMT. We all know that a small droplet of water molecule will have more than 10^{20} molecules. This enhancement will not cause any error. This algorithm is repeated for 133 molecules in the droplet.

SSMMT formation

Dynamic universe Model is n-body problem solution. Its SITA software was developed by us in early 80's by us. One

implementation is SITA software whish was running in a two floppy drive Personal Computer available at that time. It was developed such that any person who has a PC, and had little knowledge of Lotus 123 should be able to verify all the results without having to use elaborate huge main frames computers. Some of its solutions were discussed in section 7 of this paper. Many solutions/predictions came true after 10 years. See our web page for further details.

We took Dynamic Universe Model's SITA simulation software as it is, and we substituted its astronomical masses and distances values, with molecular masses and inter molecular distances values of water with other molecular values contaminations. This software is now supplemented with newly developed software for finding inter molecular HITs. We used this new set of SITA simulation software for using in this present platform. We call this new software as SSMMT.

The development of this SSMMT, is a big story where we faced lots of hurdles. This we will discuss in in some other instance.

History

We could not find any information about earlier work of earlier physicists directly on the BASIC NATURE of the force of attraction between molecules of water (inter molecular attraction forces) in Google, Bing or Academia searches. But we did find some contributors that calculated the approximate value. Similarly, we could not find the any earlier history of investigating the BASIC NATURE of state changes of water. Here we found way to corelate these states. Earlier they say that the state changes occur because of temperature and energy imparted to H_2O.

See some good explanations by Purcell [1]. IBM 704 computer was used to simulate perfectly elastic collisions between hard spheres by Alder and Wainwright [2]. Their numerical methods to solve "many-body problem" using simultaneous equations of motion gave raise to errors always by using Numerical methods. They said "this many-body problem" was solved numerically using simultaneous equations of motion. This method solves many problems in both equilibrium and nonequilibrium statistical mechanics. Probably the first simulation of matter, Gibson., *et al*. simulated radiation damage of solid copper by using a Born–Mayer type of repulsive interaction along with a cohesive surface force. 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. The spectrum of the velocity autocorrelation function shows a broad maximum in the frequency region $\omega = 0.25\ (k_B T/\hbar)$". He used a system of 864 particles interacting with a Lennard-Jones potential and obeying classical equations of motion. These are some of the N-body problem type solutions about 60 years back [3-13].

Mathematical background for 'Savitri Subbarao Multi Molecule Theory' or SSMMT:

We will use the equations presented in paper in Journal of Molecular sciences by us (2020) here using this (SSMMT). Readers may kindly note that this set of mathematics and software were used in many places. So here we show only equations:

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 systems, ensembles, aggregates, and conglomerations etc., 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, external to its system of N point masses.

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.

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

The remaining derivation of Dynamic Universe Model is available in many earlier papers, for example see our paper in 2019, if you want I will reproduce it 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 (20) and (23).

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

This work can be extended to still higher levels in a similar way.

The Equation 3 is the main powerful equation, which gives many results that are not possible otherwise today. This mathematics used here is relatively simple and straightforward. For all the mathematics, and the Excel based software, details are explained in the three books published by the author [14,15].

A point to be noted here is that the Dynamic Universe Model never reduces to General relativity on any condition. It uses a different type of mathematics based on Newtonian physics. This mathematics used here is simple and straightforward. As there are no differential equations present in Dynamic Universe Model, the set of equations give single solution in x y z Cartesian coordinates for every point mass for every time step. All the mathematics and the Excel based software details are explained in the three books published by the author In the first book, the solution to N-body problem-called Dynamic Universe Model (SITA) is presented; which is singularity-free, inter-body collision free and dynamically stable. The Basic Theory of Dynamic Universe Model published in 2010. The second book in the series describes the SITA software in EXCEL emphasizing the singularity free portions. This book written in 2011 explains more than 21,000 different equations. The third book describes the SITA software in EXCEL in the accompanying CD/DVD emphasizing mainly HANDS ON usage of a simplified version in an easy way. The third book is a simplified version and contains explanation for 3000 equations instead of earlier 21000 and this book also was written in 2011. Some of the other papers published by the author are available at references (2014, 2015). All the papers by the author are available at his webpage.

Inter molecular distances, inter molecular hits and distance factor (DF)

Let's take the colloid case in SSMMT calculations as discussed in the above Mathematical background section. We allow some iterations of calculations to happen. In every iteration of calculations, the positions of molecules will change. This happens due to the movements of all the molecules due to mutual Newtonian gravitational attraction forces. We can take any iteration result for our further analysis purposes. This iteration should be a stable one after sone initial disturbances. This iteration can be any particular one. No separate screening or selection process is required.

From the above selected iteration results, we will collect a set of 3 dimensional molecular positions, velocities and accelerations, and we will calculate inter molecular distances.

What we will do now is to change all these inter molecular distances proportionally in accordance with a Distance Factor or DF. Here we don't want to disturb the structure of We will take all the set of distances as defined in the colloid as for a Distance factor 1 or simply DF = 1. Then we will multiply this set of inter molecular distances with the DF whose value we will change manually from 0.02 to 90000. With every value of DF, we will plot addresses of hitting molecule- pairs in a designated range in Excel of 133 Row X 133 columns. We named this range as "Inter_mol_Hits". We will store the address of hitting pair of molecules in the appropriate address location in that range.

Then we will collect a screen capture 133 Row X 133 columns after zooming out appropriately to fit in a single screen for that DF value. All these screen shots are presented below after trimming the unnecessary portions. All these are depicted in next section below….

Screen Captures for different values of DFs

Figure 1: A sample screen capture can be seen here with all the inter molecular hits. If you enlarge this capture picture, you will find lots of rectangular dots, which are made up of some letters. Each of such letter combination indicates the address of two molecules which hit together or such molecules which had a hit together and are going apart after the hit. Here in this capture the background of the triangular pattern was shown as grey colour to have clear view of total range under consideration. All the later captures were snipped to grey colour area only to show all the inter molecular hits happened in that particular situation of DF value.

Figure 2: Above are Ice states for sure as all columns are full, i.e., DF 0.02 to 0.08.

Figure 3.1: This screen shot is for DF = 0.09. We see Blanks in col CT, and in Col CU Blanks from 20 to 132 rows. Please note that in the 132nd row a single blank is located in three columns viz., FH FY HM. We will use Excel method of showing the column numbers. As the memory length is limited, we made these figures small. This Figure can be enlarged to see the full details.

Figure 3.2: This screen shot is for DF = 0.1, Exactly same as above for DF = 0.09. We see Blanks in col CT, and in Col CU Blanks from 20 to 132 rows. Please note that in the 132nd row a single blank is located in three columns viz., FH FY HM. We will use Excel method of showing the column numbers. As the memory length is limited, we made these figures small. This Figure can be enlarged to see the full details.

Figure 3.3: This screen shot is for DF = 0.11. We see Blanks in col CT, and in Col CU Blanks from 20 to 132 rows. Please note that in the 132nd row a single blank is located in five columns viz., FH, FX, FY, GI, HB & HM.

Figure 3.4: This screen shot is for DF = 0.12. We see Blanks in col CT, and in Columns CU & DC Blanks from 20 to 132 rows. Please note that in the 132nd row a single blank is located in eleven columns viz., FE, FH, FM, FX, FY, GI, GN, GT, HB, HG & HM.

Figure 3.5: This screen shot is for DF = 0.13. We see Blanks in col CT, and in Columns CU & DC Blanks from 20 to 132 rows. Please note that in the 132nd row a single blank is located in 132 blank 19 columns.

Figure 3.6: This screen shot is for DF = 0.15. We see Blanks in col CT, and in Columns CU & DC Blanks from 20 to 132 rows. Please note that in the 132nd row a single blank is located in 132 blank 32 columns.

Figure 3.7: This screen shot is for DF = 0.175. We see Blanks in col CT, and in Columns CU & DC Blanks from 20 to 132 rows. Please note that in the 132nd row a single blank is located in 132 blank 44 columns.

Figure 4.1: This screen shot is for DF = 0.3. We see Blanks in col CT, and in Columns CU & DB DC Blanks from 20 to 132 rows. Please note that many full column hits and partial column hits.

Figure 4.2: This screen shot is for DF = 0.45. We see 4 Full Column hits and many partial column hits.

Figure 4.3: This screen shot is for DF = 0.5. We see 10 Full column hits and many partial column hits.

Figure 4.4: This screen shot is for DF = 0.9. We see 9 Full column hits and many partial column hits.

Figure 5.1: This screen shot is for DF = 0.9. We see 8 Full column hits and many partial column hits.

Figure 5.2: This screen shot is for DF = 1. We see 8 Full column hits and many partial column hits.

Figure 5.3: This screen shot is for DF = 1.1. We see 8 Full column hits and many partial column hits.

Figure 5.4: This screen shot is for DF = 1.2. We see 8 Full column hits and many partial column hits.

Figure 5.5: This screen shot is for DF = 1.5. We see 8 Full column hits and many partial column hits.

Figure 6.1: This screen shot is for DF = 3. We see 7 Full column hits and many scattered hits.

Figure 6.2: This screen shot is for DF = 4.5. We see 7 Full column hits and 50 scattered hits.

Figure 6.3: This screen shot is for DF = 5. We see 6 Full column hits and low scattered hits.

Figure 6.4: This screen shot is for DF = 6. We see 6 Full column hits and 14 hits + some scattered hits.

Figure 6.5: This screen shot is for DF = 7.5. We see 6 Full column hits and 12 hits + 12 scattered hits.

Figure 7.1: This screen shot is for DF = 9. We see 6 Full column hits and 18 hits.

Figure 7.2: This screen shot is for DF = 10 We see 6 Full column hits and very low number of hits.

Figure 7.3: This screen shot is for DF = 15. We see 6 Full column hits and 13 hits.

Figure 7.4: This screen shot is for DF = 30. We see 6 Full column hits and 12 hits.

Figure 7.5: This screen shot is for DF = 45. We see 6 Full column hits and 9 hits.

Figure 7.6: This screen shot is for DF = 50. We see 6 Full column hits and 8 hits.

Figure 7.7: This screen shot is for DF = 60. We see 6 Full column hits and 8 hits.

Figure 7.8: This screen shot is for DF = 75. We see 6 Full column hits and 8 hits.

Figure 7.9: This screen shot is for DF = 90. We see 6 Full column hits and 8 hits.

Figure 7.10: This screen shot is for DF = 100. We see 6 Full column hits and 8 hits.

Figure 7.11: This screen shot is for DF = 150. We see 6 Full column hits and 8 hits.

Figure 7.12: This screen shot is for DF = 300. We see 6 Full column hits and 8 hits.

Figure 8.1: This screen shot is for DF = 450. We see 3 Full column + 3 scattered column hits and 6 hits.

Figure 8.2: This screen shot is for DF = 500. We see 3 Full column hits + 3 scattered column hits and 4 hits.

Figure 8.3: This screen shot is for DF = 600. We see 2 Full column hits + 1 scattered column hits and some scattered hits.

Figure 8.4: This screen shot is for DF = 750. We see 2 Full column hits + 1 column with 10 scattered hits and 4 hits.

Figure 8.5: This screen shot is for DF = 900. We see 1 Full column hits + 1 scattered column hits and 4 hits.

Figure 8.6: This screen shot is for DF = 1000. We see 1 Full column hits + 1 scattered column hits and 2 hits.

Figure 9.1: This screen shot is for DF = 3000. We see 1 scattered column hits and 2 hits.

Figure 9.2: This screen shot is for DF = 4500. We see 1 scattered column hits and 1 hit.

Figure 9.3: This screen shot is for DF = 5000. We see 1 scattered column hits and 2 hits

Figure 9.4: This screen shot is for DF = 6000. We see 1 much scattered column hits and 2 hits.

Figure 9.5: This screen shot is for DF = 7500. We see 1 column of 3 hits.

Figure 9.6: This screen shot is for DF = 9000. We see 1 hit.

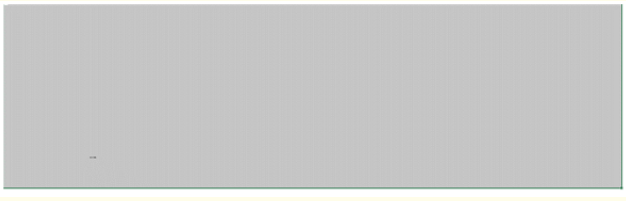

Figure 9.7: This screen shot is for DF = 10000. We see 1 hit.

Figure 10: This screen shot is for DF = 15000 to DF = 90000. We see it is totally Blank.

Observations on screen captures

The above screen shots show the different states of H_2O depending on inter molecular distances. These screen shots were based on different Distance factors (DFs) ranging from 0.02 to 90000. They show a gradual transition of change of states of (H_2O) water as a function of Distance factor. We used the term H_2O as 'water' is also another state.

A sample full screen capture can be seen here with all the inter molecular hits in figure 1. If one enlarges this capture picture, one will find lots of rectangular dots, which are made up of some letters. Each of such letter combination indicates the address of two molecules which hit together or such molecules which had a hit together and are going apart after the hit. Here in this capture the background of the triangular pattern was shown as grey colour to have clear view of total range under consideration. All the later captures were snipped to grey colour area only to show all the inter molecular hits happened in that particular situation of DF value.

We can observe 'Ice' states for DF values equal to 0.02 to 0.08 in Figure 2. Here we see all columns are full of Inter molecular Hits.

The screen captures in figure 3.1 to figure 3.6 also show the Ice states for DF values from 0.1 to 0.175. We can observe in first column below 20 are all blanks and bottom-line pitting started.

The screen capture in figure 4.1. to figure 4.4. show 'Ice + some water' states and we can see ice started melting. We can observe Missing first column of hits and some pitting on overall triangle. In these states first column are all blanks and bottom line, second and third column pitting started. These are for DF values from 0.3 to 0.8.

The screen capture in figure 5.1. to figure 5.5. are 'water + some ice' states and we can see ice melted. Common factor is '8 full columns of hits'. We can also observe Missing first column of hits and with 4 hits or above in next two columns. Pitting in 4^{th} column is increased gradually as well as pitting on the overall triangle. These are for DF values 0.9 to 1.5.

The screen capture in figure 6.1. to figure 6.5 are 'water + much less Ice' states we can see ice melted. Common factor is '6 full columns of hits'. We can see water is getting evaporated. Common factor is '6 full columns of hits.' We can also observe Missing first two columns of hits and with 6 hits or above in next three columns. Pitting on the overall triangle is increased gradually. These are for DF values 3 to 7.5.

The screen capture in figure 7.1. to figure 7.12 are 'water' states we can see water is getting evaporated. Common factor is '6 columns of full hits'. We can also observe Missing first two columns of hits and with 6 hits or above in next three columns. Pitting on the overall triangle is increased gradually to full blank after the 6 columns. These are for DF values 9 to 300.

The screen capture in figure 8.1. to figure 8.6. are 'water in evaporation' states. The earlier common factor of '6 full columns of hits' was slowly disintegrated and vanished. We can see water is getting evaporated. In other words, pitting on the 6 columns of hits is increased gradually. These are for DF values 450 to 1000.

The screen capture in figure 9.1. to 9.7. are 'water fully evaporated' states. The only common factor of 'one column of hits' was slowly disintegrated and vanished. We can see water got getting evaporated fully. These are for DF 5000 to 10000.

The screen capture in figure 10. is 'water vapour fully scattered' state for DF values 15000 to 90000. All these screen captures are blank without any hits. The distances between molecules so high, it becomes almost impossible to for any molecule to hit another.

This way these screen captures for DF values 0.02 to 90000 show gradual transmission of states of water as function of inter molecular distances.

Creation of Screen Captures

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.

SSMMT vs sita simulations

Basic difference between SSMMT and Sita Simulations are the values of masses and distances between the masses.

Mathematical frame work is exactly the same. Use the molecular masses and inter molecular distances for SSMMT in SITA simulations this will become SSMMT.

SITA solution can be used for solving presently unsolved problems in many situations like …

- Prediction of large number of Blue-shifted Galaxies (>5) at 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 Energy level.

SSMMT simulations

We use SSMMT Simulations for finding the Combined Vector Force using Newtonian Gravitation as Binding Force Between H_2O Molecules for explaining the Basic Nature of Inter Molecular Attraction Forces and to explain the formation of Three States of Water using SSMMT at Nanoparticle level.

This is totally a new application at H_2O Molecules level.

This problem was never explored by anyone in the world. Attempts were made by many to measure the value of the force in the last 3 centuries, but no one attempted to find the basic nature of this force. This problem was never attempted.

We already presented/published many papers on SSMMT for applications of Brownian motion.

Conclusion

We can safely conclude the inter molecular forces 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, we used SITA forces for explaining the Basic Nature of Inter Molecular Attraction Forces.

Now we can safely conclude, Newtonian Gravitation is necessary, appropriate and sufficient for explaining the basic nature of inter molecular attraction forces between H_2O molecules as defined by Multi Molecule theory. We already know SSMMT uses collective gravitational attraction all the molecules on any single molecule in the collection of molecules.

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.

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helping me pass through all the hurdles to attain the victory of solving this problem. I thank God Vishnu for giving the courage to solve this problem.

Data Availability

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

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