Introducing an Alternative Mathematical Model for Tracing the flow of Internal Molecular Frequency Distribution and Predicting the Pattern Exact Diffusion at Boundary of Fluid Droplet

Md. Tasfiq Rahman and Chinmoy Mandal Shishir

November 7, 2020

Introducing an Alternative Mathematical Model for Tracing the flow of Internal Molecular Frequency Distribution and Predicting the Pattern Exact Diffusion at Boundary of Fluid Droplet

Md. Tasfiq Rahman [1], Chinmoy Mandal Shishir[2]

[1]*(Electrical & Electronic Engineering, Bangladesh University of Engineering and Technology, Bangladesh)*

[2]*(Electrical & Electronic Engineering, Ahsanullah University of Science and Technology, Bangladesh)*

Author's e-mail: dehan.drmc@gmail.com

Abstract:

Analyzing the complex behavior of fluid droplet is still an ongoing research topic throughout the world. A crystal-clear understanding of such natural event may lead us to give more accurate prediction of the pattern of Faraday wave. Moreover, we can utilize this concept in our blood circulation system to develop a system for early disease detection using fluid droplet. In summary, it will enable us to organize such a co-ordinate system where a certain molecule in the drop will act as its reference point and the reference can be controlled from a distance. The first part to organize such system would be to study how the flow of inter molecular frequency of a fluid droplet. This internal frequency distribution causes the change in shape at the boundary of a certain droplet. Such rapid and periodic change of water droplet was observed in 2015 on a superhydrophobic surface (published in Nature). Its focus was to study the movement of the center of mass as fluid trampoline. Here our main objective would be to observe how the boundary of different position of the boundary of water droplet is changed with time on a superhydrophobic surface. It can give an insight about the change of boundary position (and internal frequency distribution) of water droplet in a hydrophilic and mixed environment (blood). Our methodology can be divided into four steps. First step is to take the video of a certain water droplet on different surface. Second step was to observe the video in slow motion and find out the mentionable shape change of water boundary. Third step is to fit a suitable equation whose plot can be perfectly matched with the shape of water droplet and change of different coefficient in the equation gives different real observed shape of vibrating water droplet. Last step is to analyze the equation to make a link of the variable in our proposed equation with the variable of the physical world. Following this methodology, we have observed that change of water boundary on a superhydrophobic surface comes from 4^{th} order polynomil equation of two-dimensional position with sinusoidal term. Later our finding was more complicated and accurate. It has also been observed that center of mass and elasticity may have effect on the scattering of intermolecular frequency.

Key Word: Microfluid, Superhydrophobic, Frequency, Weber number, Molecular dynamics

I. Introduction

A study has shown that droplet of microfluid shows turbulent shape on superhydrophobic space Thomas et al 2015 [1]. In this literature many physical properties regarding this characteristic has been explained. The shape of droplet was calculated with the approach of machine learning Jian et al [2]. We have used the result of [1] but numerical approach would be taken to extract inner information of a fluid droplet.

After trial and error effective manual equation has been formed through which prediction of future shape of a certain fluid droplet can be given at a certain condition. In the work of [1], the trajectory of the droplet was considered within the height. This was divided into two categories. One dimensional motion during levitation and mass spring system during the impact with the superhydrophobic surface. Here Webber number has been considered as the factor of droplet shape and stiffness. But this cannot give a sense of what is happening inside. So, after generating the equation of the shape, the coefficients were also found as the function of time. Each coefficient brings valuable information. If increase of one coefficient change the shape of a certain portion of the water droplet, it would be regarded as the movement of molecules in that certain region. It also affects the position of other molecules and thus there would be a rational dynamic process. Using our numerical approach and interpretation of each co-efficient, we can easily navigate the position of a certain molecule. Moreover we can also approximate the direction of its movement at a certain time. This way of study may make molecular dynamics based simulation system more efficient.

II. Tools and Method

This experiment has been confined to two-dimensional analysis. Here the tools are mainly software based. These are:

1) FastStone Capture
2) Desmos
3) Microsoft Excel
4) MATLAB

Our first approach was to extract certain portion of the following video [3] . This portion was from 1 minute 41 second to 1 minute 53 second. During the time of capturing this video, we paused it several times so that quite steady state pattern of the droplet can be observed from the real turbulent phenomenon. The link of our captured video has been given in the following [4].

Again, taking screenshot of several consecutive patterns of this video, we have noticed 21 different patterns of water droplet.

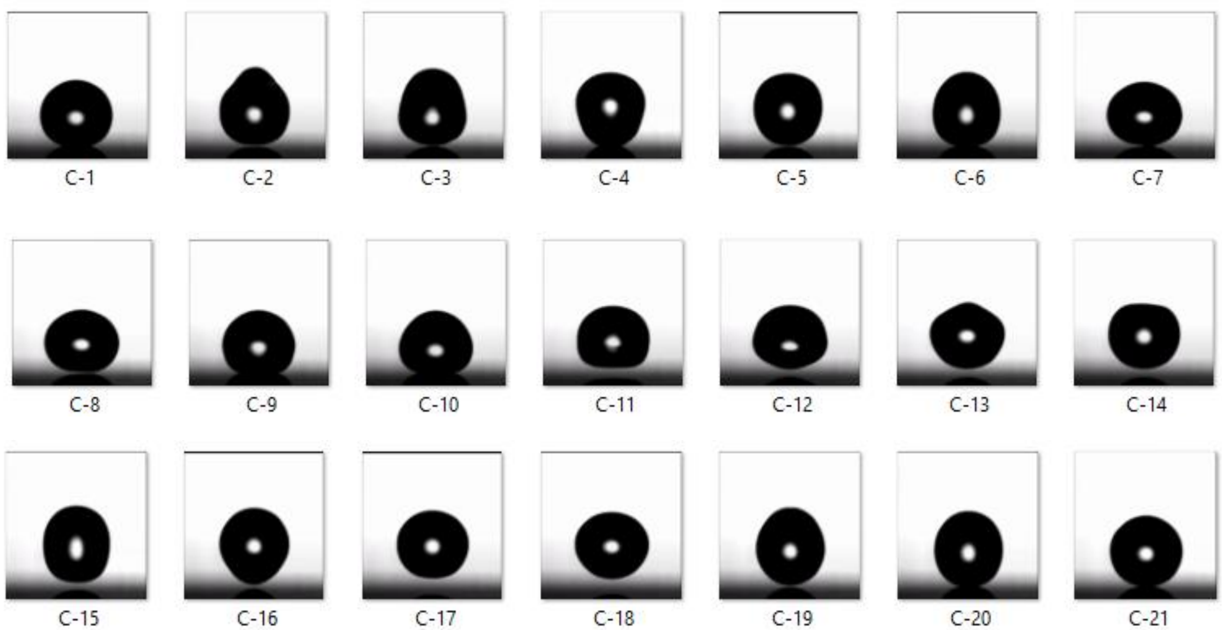
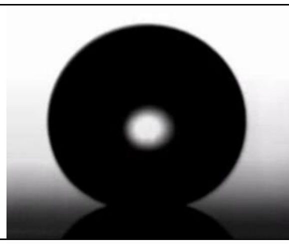
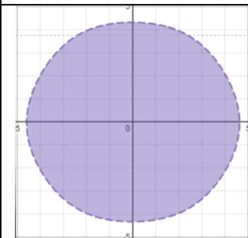
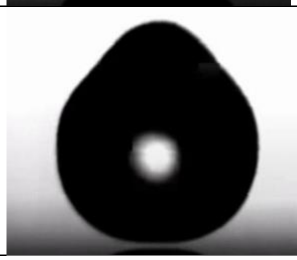
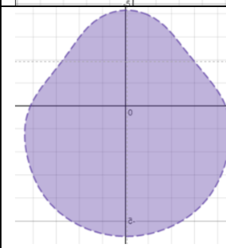
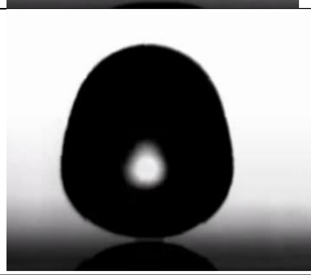
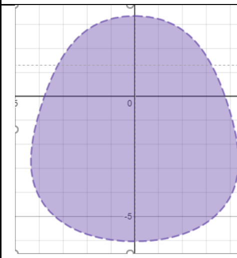
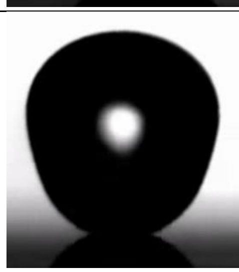
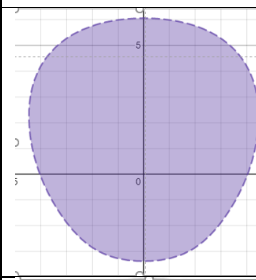
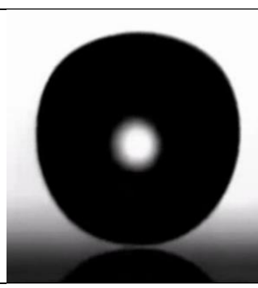
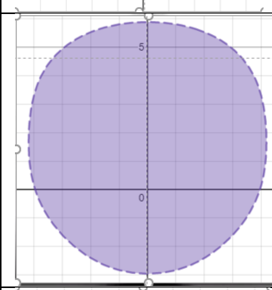
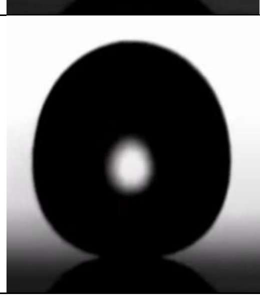
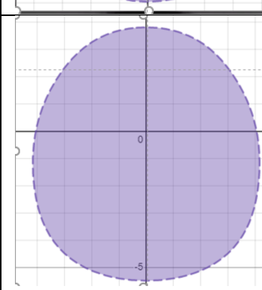


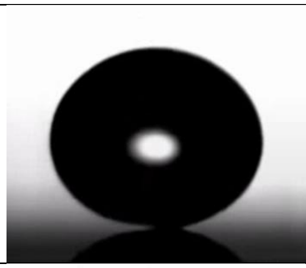
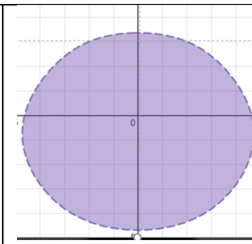
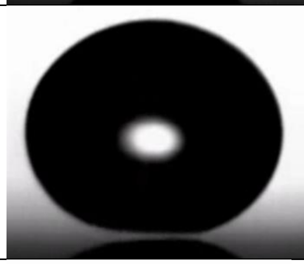
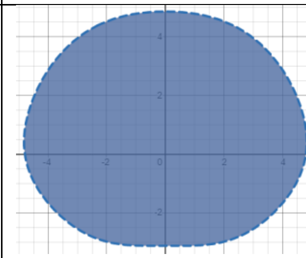
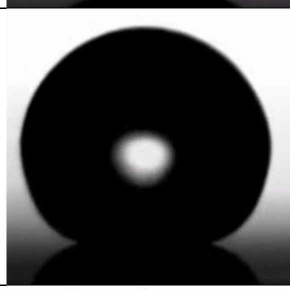
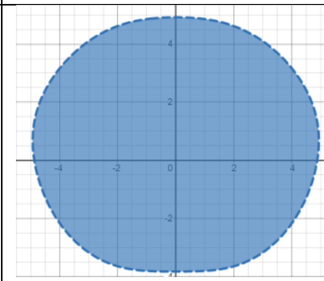
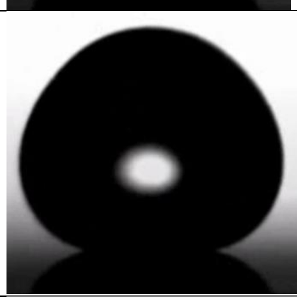
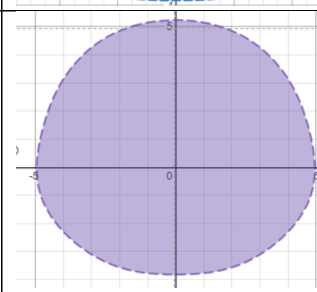
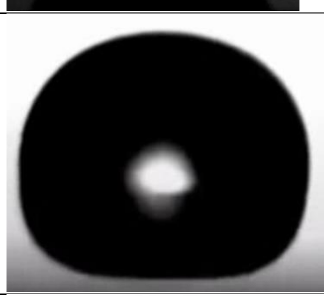
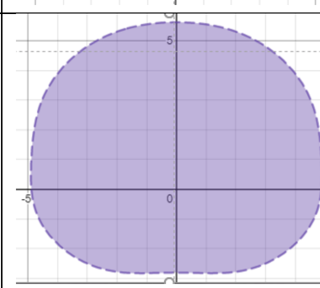
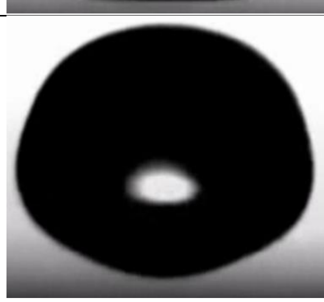
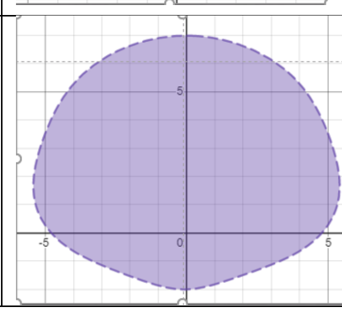
Fig 1: Twenty one different patterns from one bouncing cycle

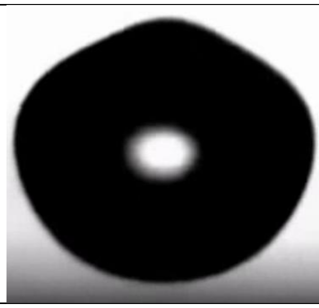
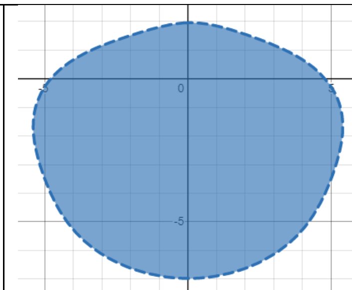
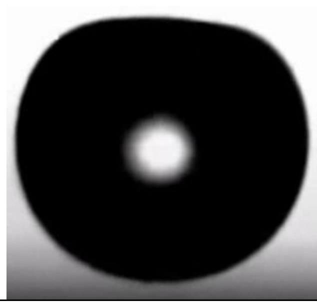
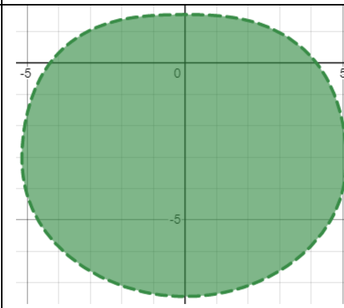
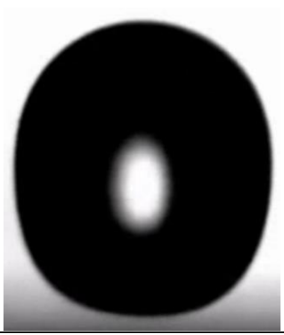
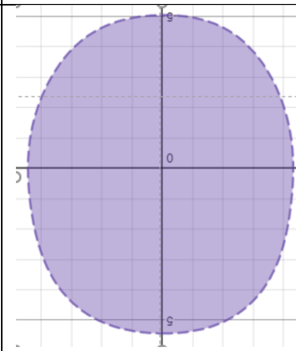
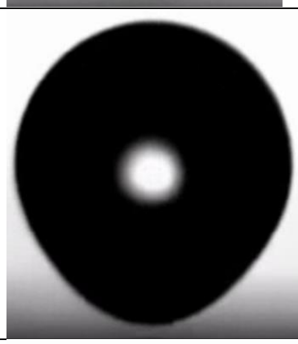
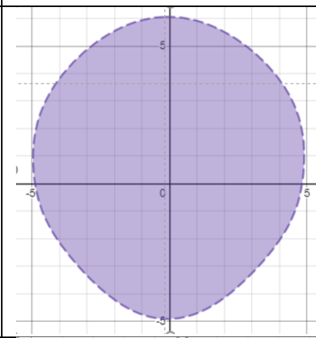
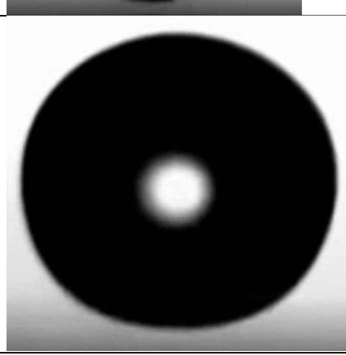
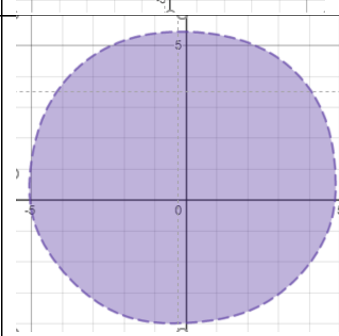
Then we started forming equation for the corresponding pattern trying to fit it as accurate as possible.

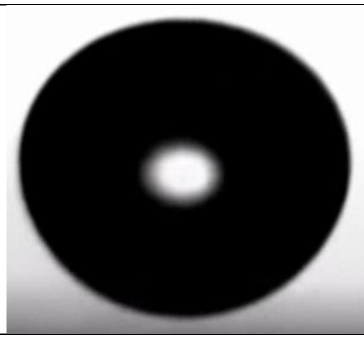
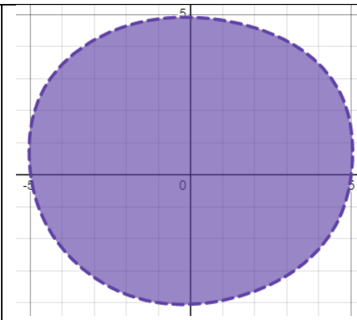
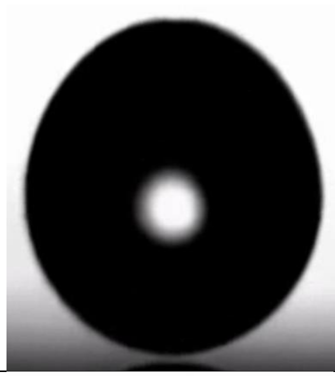
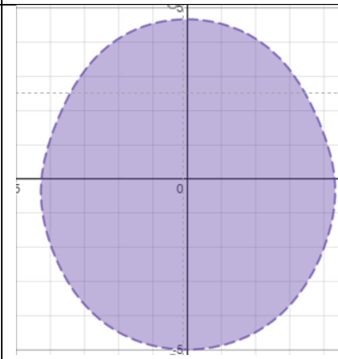
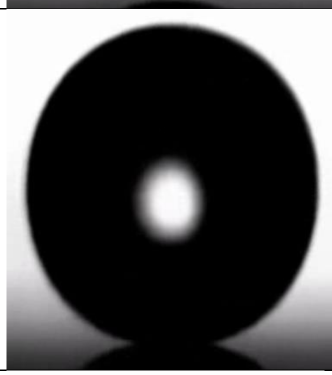
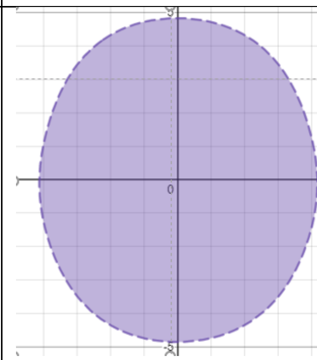
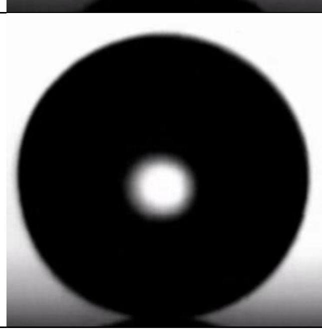
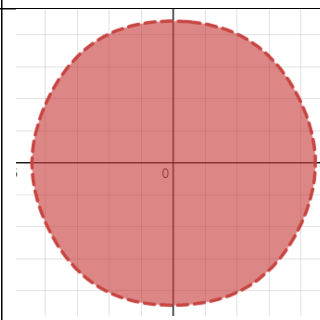
After the process of trial and error, we have formed 224 equations and plotted their corresponding graphs using Desmos. Finally the best fitted graph with their corresponding equation has been given below.

Table 2.1: Generated equation from the shape of droplet

No. of pattern	Observed Shape	Equation	Plot (2D)
1		$0.094x^4 + 0.305y^4 + 0.43x^2y^2 + 0.7x^2 - 3.3y^2 + 0.4sinx + 7.7cosx + 0.6siny - 3.6cosy - 0.1x - 0.3y - 53.7 = 0$	
2		$0.105x^4 + 0.29y^4 + 0.31x^2y^2 + 1.3x^2 - 5y^2 + 0sinx - 7cosx + 2.4siny - 10cosy + 1x + 13y - 50 = 0$	
3		$0.154x^4 + 0.29y^4 + 0.31x^2y^2 + 1.7x^2 - 5.7y^2 + 0sinx + 3.4cosx - 4siny + 21cosy - 0x - 0.3y - 50 = 0$	
4		$0.154x^4 + 0.29y^4 + 0.333x^2y^2 + 1.3x^2 - 5.7 + 0sinx + 5cosx + 0.5siny - 5cosy - 0x - 21y - 29 = 0$	
5		$0.154x^4 + 0.29y^4 + 0.356x^2y^2 + 2.1x^2 - 4.6y^2 + 0sinx + 3.4cosx + 2.6siny - 10.6cosy - 0x - 21y - 57.6 = 0$	
6		$0.145x^4 + 0.294y^4 + 0.356x^2y^2 + 2.4x^2 - 4y^2 + 0sinx + 4.6cosx - 2siny - 6.7cosy - 0x + 13.8y - 68.7 = 0$	

7		$0.104x^4 + 0.31y^4 + 0.395x^2y^2 + 0.2x^2 - 2y^2 + 0sinx + 3.4cosx + 3.8siny - 4.6cosy - 0x + 11y - 61.8 = 0$	
8		$0.104x^4 + 0.327y^4 + 0.593x^2y^2 + 0.3x^2 - 2.5y^2 + 0sinx + 13cosx + 5.2siny - 0.3cosy - 0x - 14y - 63.2 = 0$	
9		$0.124x^4 + 0..229y^4 + 0.527x^2y^2 + 0x^2 - 0.9y^2 + 0sinx + 14.2cosx - 1.4siny + 8.5cosy - 0x - 10y - 80.8 = 0$	
10		$0.122x^4 + 0.226y^4 + 0.541x^2y^2 + 0x^2 - 1.4y^2 + 0sinx + 10.2cosx + 11.6siny + 5cosy - 0x - 10.3y - 80.8 = 0$	
11		$0.11x^4 + 0.229 + 0.5y^2 + 0x^2 - 1y^2 + 0sinx + 11.3cosx + 18siny + 6.7cosy - 0x - 23.4y - 71 = 0$	
12		$0.094x^4 + 0.182y^4 + 0.253x^2y^2 + 0.2x^2 - 4.1y^2 + 0.4sinx - 3cosx - 10.6siny - 9cosy + 0.1x - 24.4y - 44.8 = 0$	

13		$0.094x^4 + 0.182y^4 + 0.253x^2y^2 + 0.2x^2 - 4.1y^2 - 0.4sinx - 3cosx + 10.6siny - 9cosy - 0.1x + 24.4y - 44.8 = 0$	
14		$0.1x^4 + 0.188y^4 + 0.302x^2y^2 + 0.6x^2 - 5.4y^2 - 0.4sinx + 1.2cosx - 4.6siny - 7cosy + 0.4x + 32.7y - 34.7 = 0$	
15		$0.087x^4 + 0.19y^4 + 0.312x^2y^2 + 0.4x^2 - 4.2y^2 - 0.9sinx + 7.7cosx - 2.1siny - 1.6cosy - +0.4x + 2.1y - 35.7 = 0$	
16		$0.051x^4 + 0.17y^4 + 0.312x^2y^2 + 0.2x^2 - 4.1y^2 + 0.8sinx - 2.9cosx + 3.5siny + 2.9cosy - +0.3x - 7y - 35.7 = 0$	
17		$0.048x^4 + 0.235y^4 + 0.343x^2y^2 + 0.2x^2 - 4.3y^2 + 1sinx + 7.2cosx + 5.5siny + 0.5cosy + 0.9x - 8.6y - 35.7 = 0$	

18		$0.063x^4 + 0.332y^4 + 0.314x^2y^2 - 0.1x^2 - 5y^2 + 2sinx + 0.4cosx + 2.8siny - 0.3cosy - +0.3x - 6.7y - 37.4 = 0$	
19		$0.062x^4 + 0.305y^4 + 0.43x^2y^2 + 1.1x^2 - 5.7y^2 + 0.4sinx + 3.5cosx + 0.3siny - 3.6cosy - 0.1x + 2.7y - 36.4 = 0$	
20		$0.059x^4 + 0.305y^4 + 0.43x^2y^2 + 1.8x^2 - 5.6y^2 + 0.4sinx + 6.6cosx + 0.5siny - 3.6cosy - 0.1x - + 0.3y - 10 = 0$	
21		$0.094x^4 + 0.305y^4 + 0.43x^2y^2 + 1.1x^2 - 3.8y^2 + 0.4sinx + 7.6cosx + 0siny - 3.6cosy - 0.1x + 0.3y - 52.5 = 0$	

III Result

A common relation has been observed among these patterns. A general equation which can satisfy all the shape is given below:

$$a_{x^4}(t)x^4 + a_{y^4}(t)y^4 + a_{x^2y^2}(t)x^2y^2 + a_{x^2}(t)x^2 + a_{y^2}(t)y^2 + a_{sin(x)}(t)sinx + a_{cos(x)}(t)cosx + a_{sin(y)}(t)siny + a_{cos(y)}(t)cosy + a_x(t)x + a_y(t)y + a_{const}(t) = 0 \quad \text{......................(1)}$$

Table of Corresponding Coefficients

No	x^4	y^4	x^2y^2	x^2	y^2	sin(x)	cos(x)	sin(y)	cos(y)	x	y	constant
1	0.094	0.305	0.43	0.7	-3.3	0.4	7.7	0.6	-3.6	-0.1	-0.3	-53.7
2	0.105	0.29	0.31	1.3	-5	0	-7	2.4	-10	1	13	-50
3	0.154	0.29	0.31	1.7	-5.7	0	3.4	-4	-3	0	21	-50
4	0.154	0.29	0.333	1.3	-5.7	0	5	0.5	-5	0	-21	-29
5	0.154	0.29	0.356	2.1	-4.6	0	3.4	2.6	-10.6	0	-21	-57.6
6	0.145	0.294	0.356	2.4	-4	0	4.6	-2	-6.7	0	13.8	-68.7
7	0.104	0.31	0.395	0.2	-2	0	3.4	3.8	-4.6	0	11	-61.8
8	0.104	0.327	0.593	0.3	-2.5	0	13	5.2	0.3	0	-14	-63.2
9	0.124	0.229	0.527	0	-0.9	0	14.2	-1.4	8.5	0	-10	-80.8
10	0.122	0.226	0.541	0	-1.4	0	10.2	11.6	5	0	-10.3	-80.8
11	0.11	0.229	0.5	0	-1	0	11.3	18	6.7	0	-23.4	-71
12	0.094	0.182	0.253	0.2	-4.1	0.4	-3	-10.6	-9	0.1	-24.4	-44.8
13	0.094	0.182	0.253	0.2	-4.1	-0.4	-3	10.6	-9	-0.1	24.4	-44.8
14	0.1	0.188	0.302	0.6	-5.4	-0.4	1.2	-4.6	-7	0.4	32.7	-34.7
15	0.087	0.19	0.312	0.4	-4.2	-0.9	7.7	-2.1	-1.6	0.4	2.1	-35.7
16	0.051	0.17	0.312	0.2	-4.1	0.8	-2.9	3.5	2.9	0.3	-7	-35.7
17	0.048	0.235	0.343	0.2	-4.3	1	7.2	5.5	0.5	0.9	-8.6	-35.7
18	0.063	0.332	0.314	-0.1	-5	2	0.4	2.8	0.3	0.3	-6.7	-37.4
19	0.062	0.305	0.43	1.1	-5.7	0.4	3.5	0.3	-3.6	-0.1	2.7	-36.4
20	0.059	0.305	0.43	1.8	-5.6	0.4	6.6	0.5	-3.6	0.1	0.3	-10
21	0.094	0.305	0.43	1.1	-3.8	0.4	7.6	0	-3.6	-0.1	0.3	-52.5

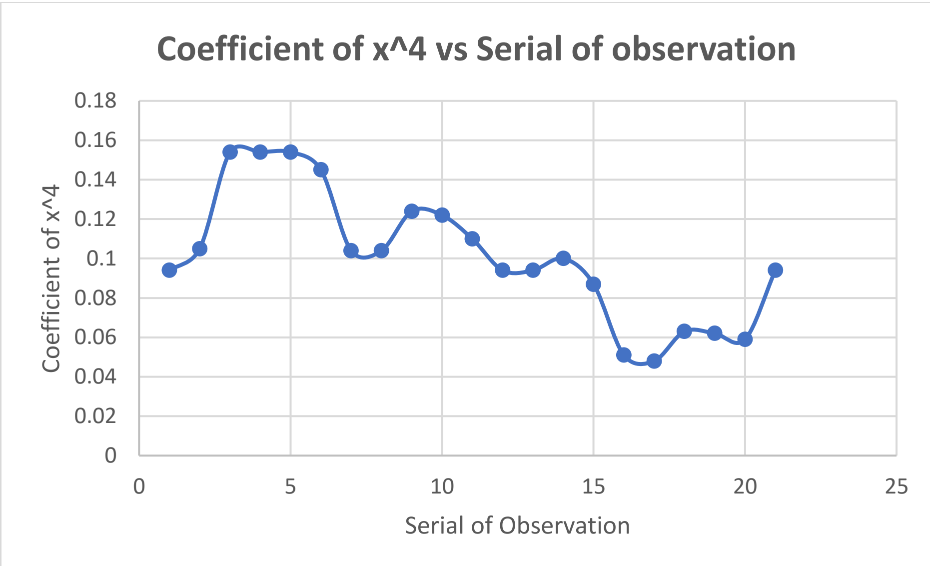
The coefficients are changing with time. To predict the displacement of a certain molecule two factors should be taken into consideration.

1) The change of coefficient of each term with respect to time.

2) The effect of each coefficient on the shape of fluid droplet

3.1. The change of coefficient of each term with respect to time:

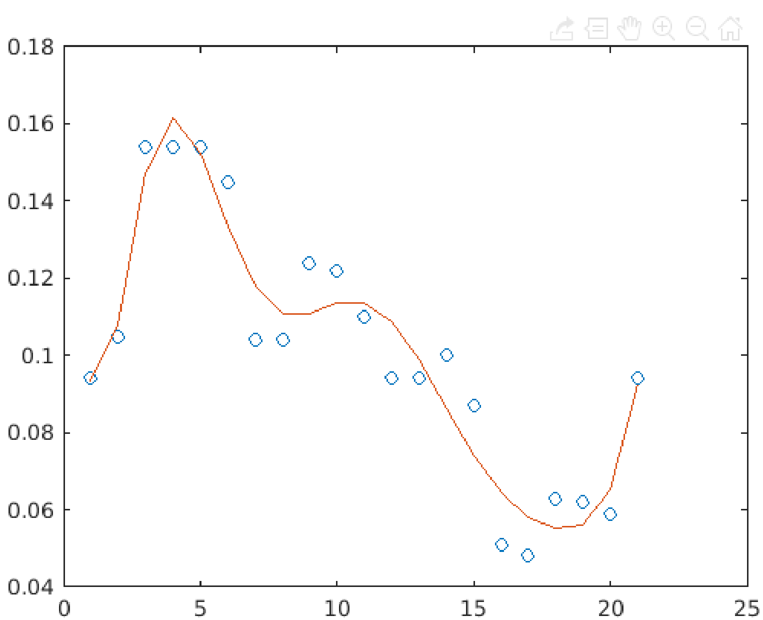
Using MS excel, best fit curve of the corresponding coefficient set of each term has been shown first. Next, an optimized equation for the corresponding dataset has been generated using the polyfit() function in MATLAB. Finally the plot of our generated equation is drawn using polyval() function.

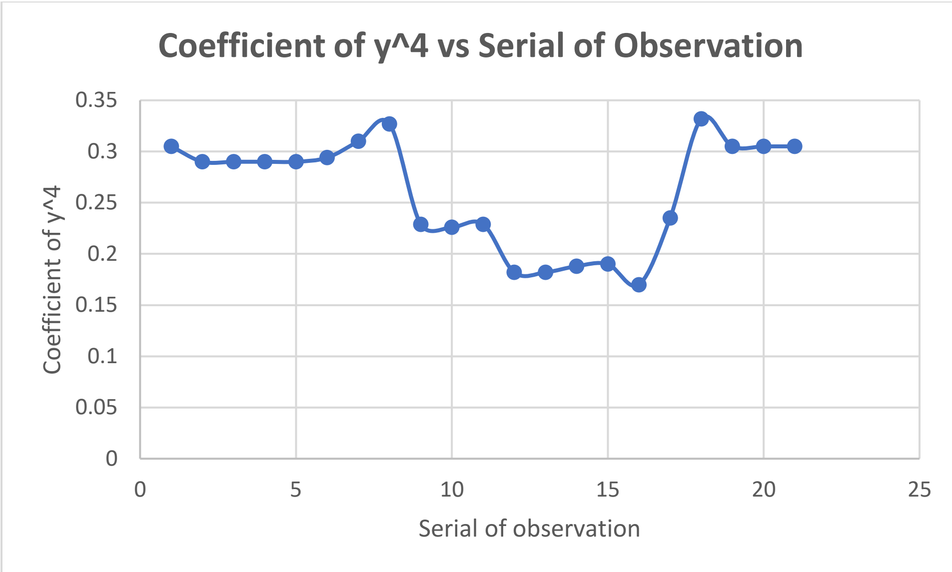


Equation:

$a_{x^4}(t) = 0.0001t^6 - 0.014t^5 + 0.014t^4 - 0.0826t^3 + 0.2577t^2 - 0.3543t + 0.2597$

Plot:

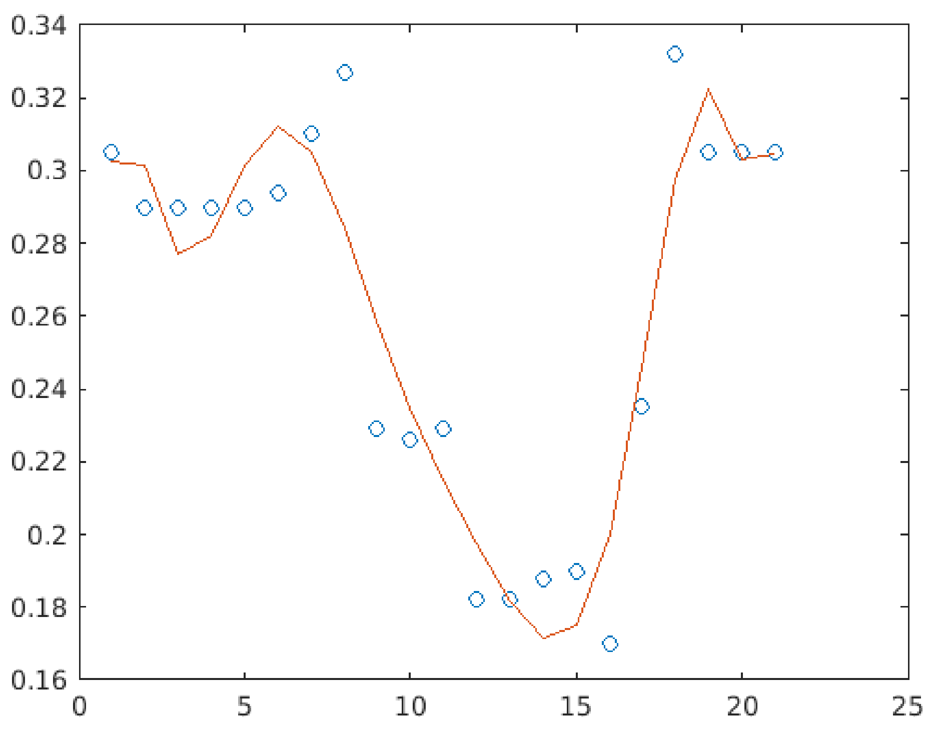


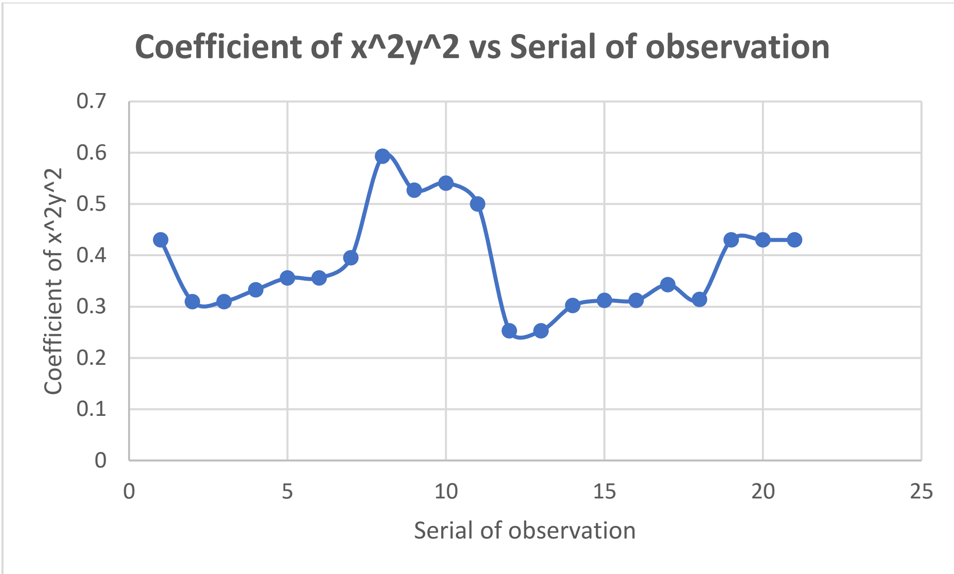


Equation:

$a_{y^4}(t)$ = -0.0003t^6 + 0.0039t^5-0.0329t^4 + 0.1630t^3-0.4471t^2 + 0.5871t + 0.0287

Plot:

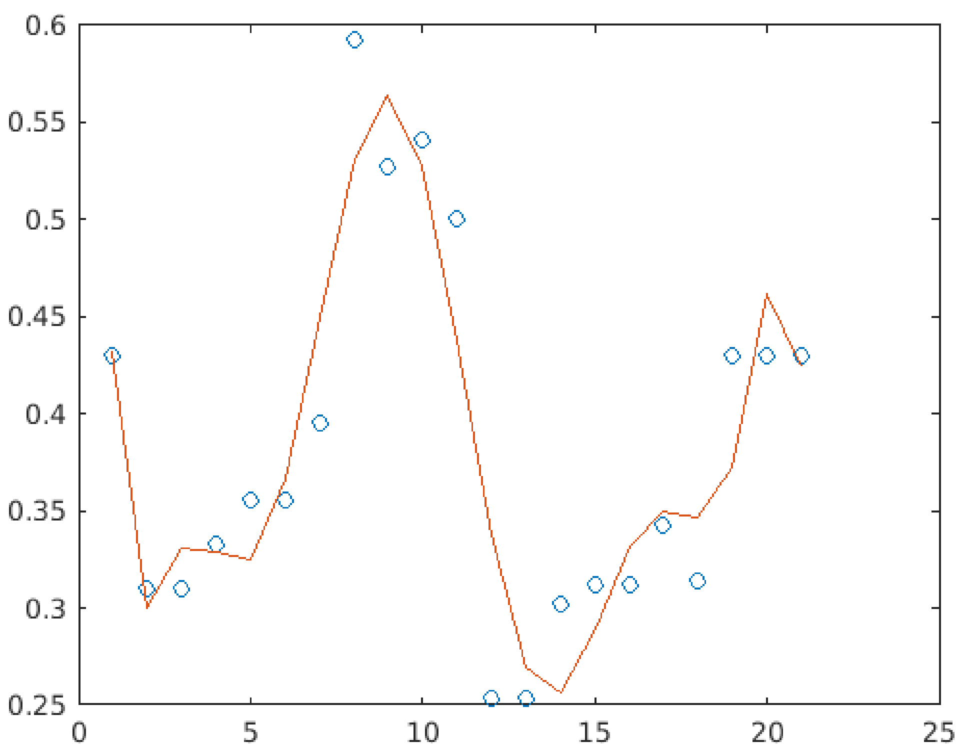


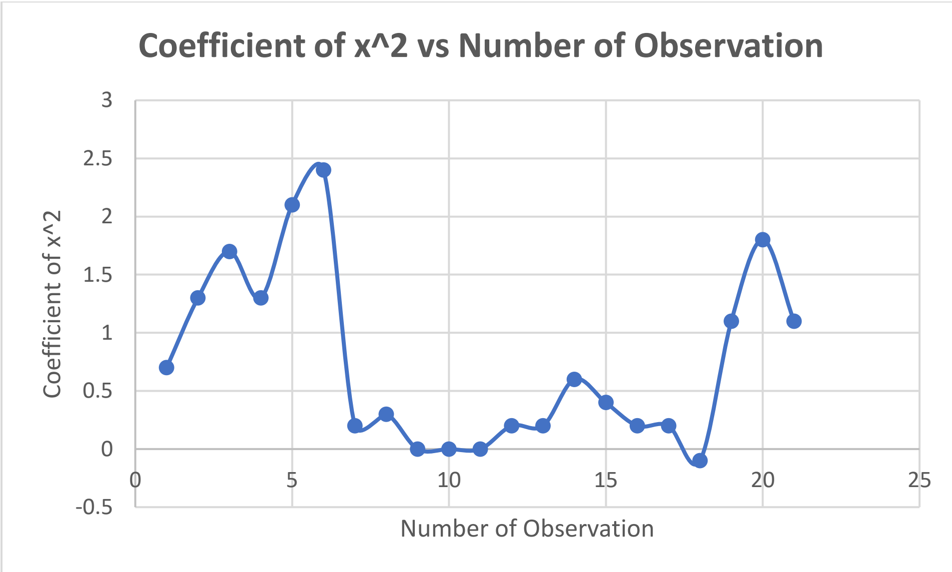


Equation:

$a_{x^2y^2}(t) = 0.11t^6 - 0.0148t^5 + 0.1209t^4 - 0.5922t^3 + 1.6536t^2 - 2.3669t + 1.6298$

Plot:

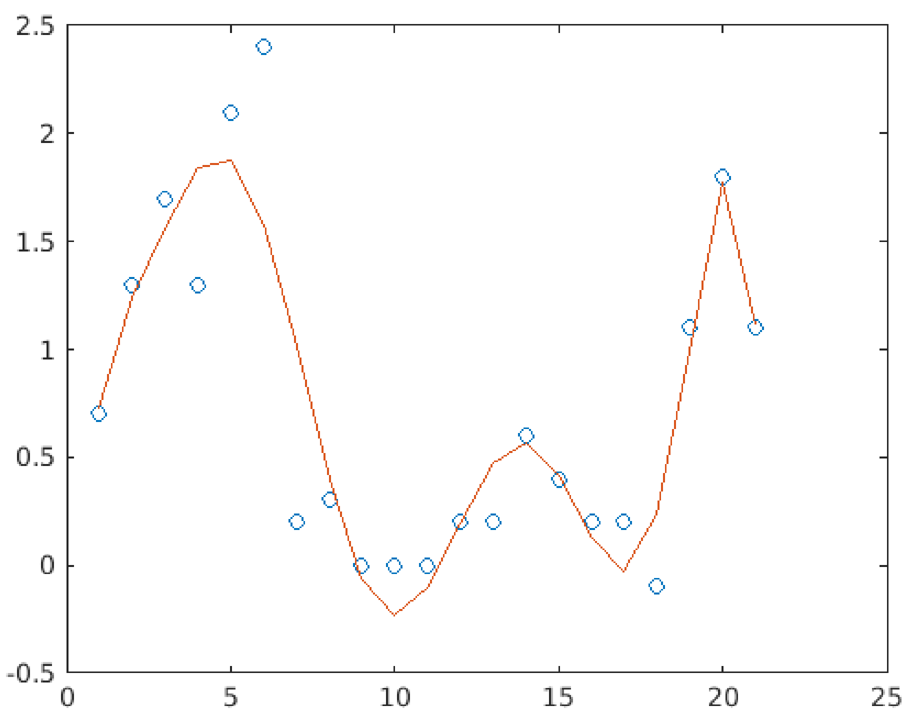


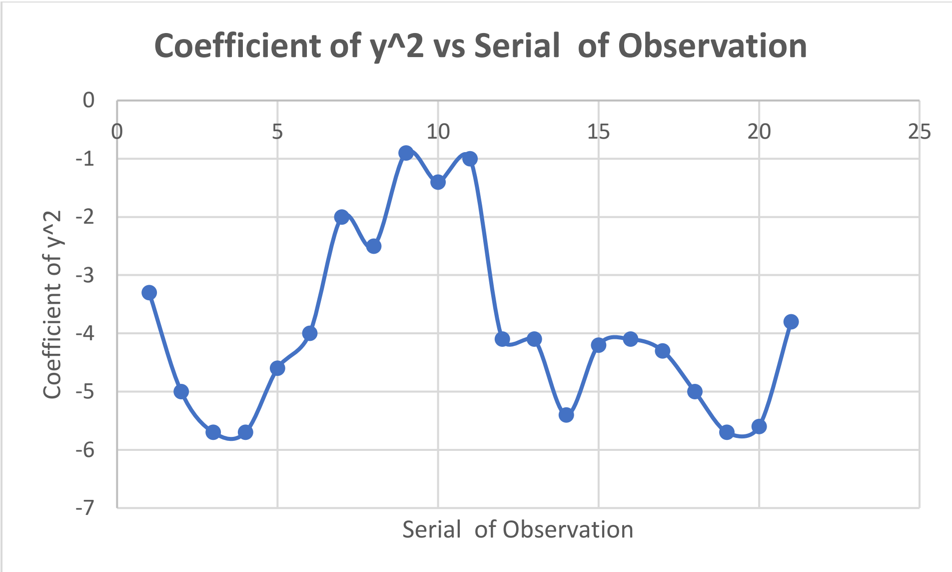


Equation:

$a_{x^2}(t)$ = 0.0001t^7-0.0019t^6 + 0.00265t^5-0.2174t^4 + 1.0137t^3-2.6317t^{2}3.8631t-1.3284

Plot:

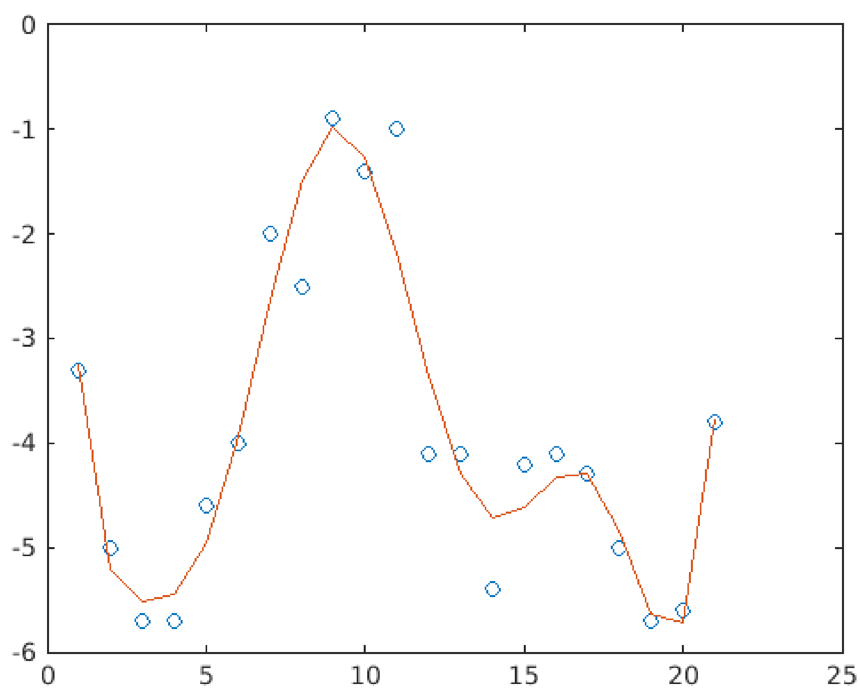


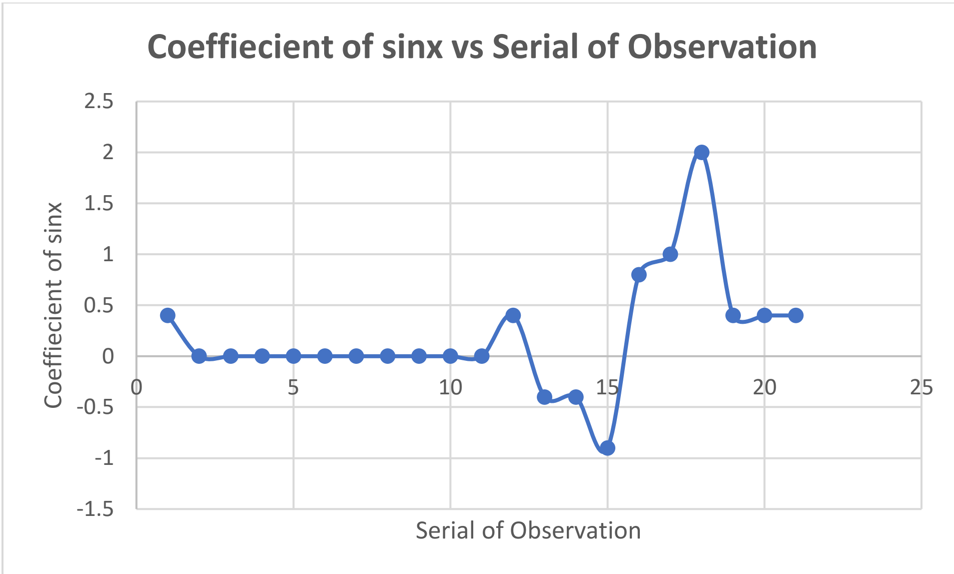


Equation:

$a_{y^2}(t)$ = -0.0003t^7 + 0.0069t^6-0.0943t^5+0.7703t^4-3.765t^3 + 10.8389t^2-17.1608t + 6.1570

Plot:

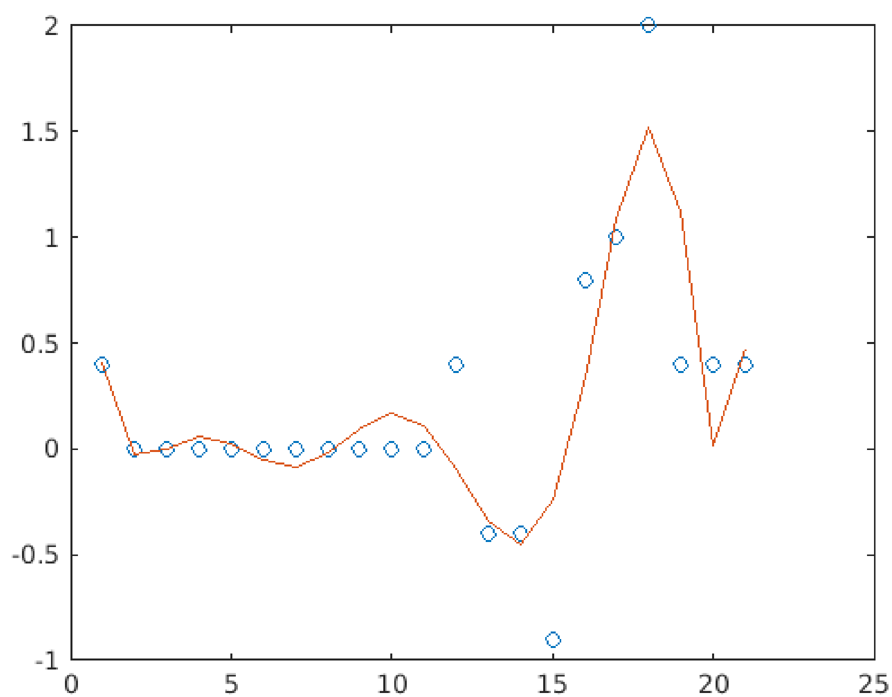


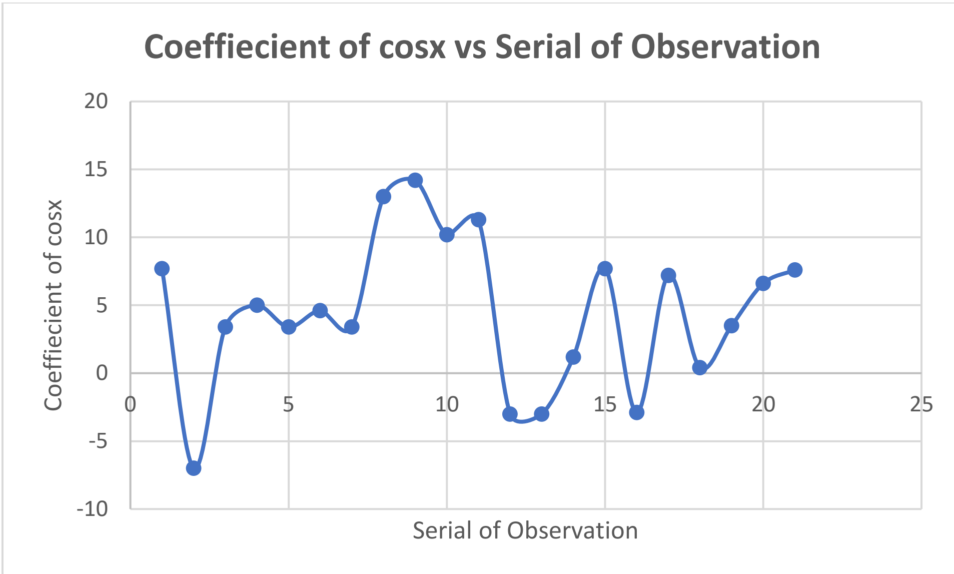


Equation:

$a_{sin(x)}(t)$ = 0.0001t^7-0.011t^6 + 0.0092t^5-0.0285t^4-0.0974t^3 + 0.9761t^2-2.4827t + 2.0348

Plot:

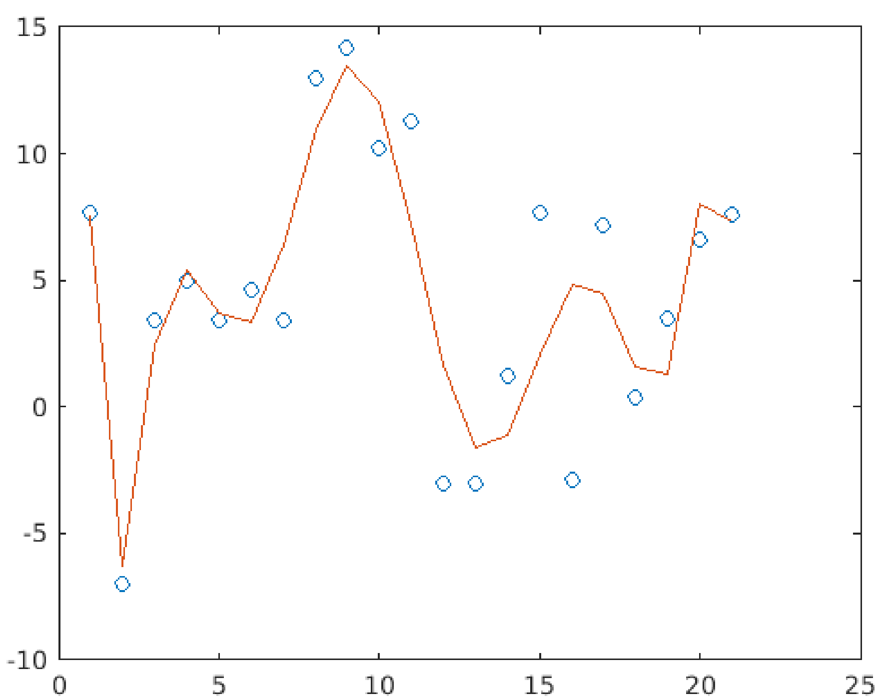


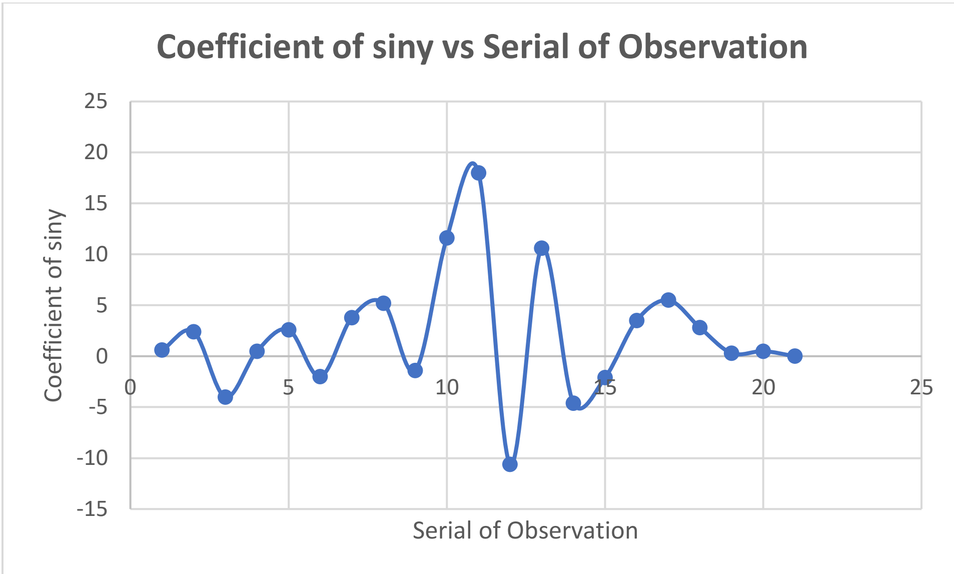


Equation:

$$a_{cos(x)}(t) = 0.001t^8 - 0.0046t^7 + 0.1065t^6 - 1.4858t^5 + 12.6927t^4 - 65.3812t^3 + 192.0095t^2 - 282.7107t + 152.3213$$

Plot:

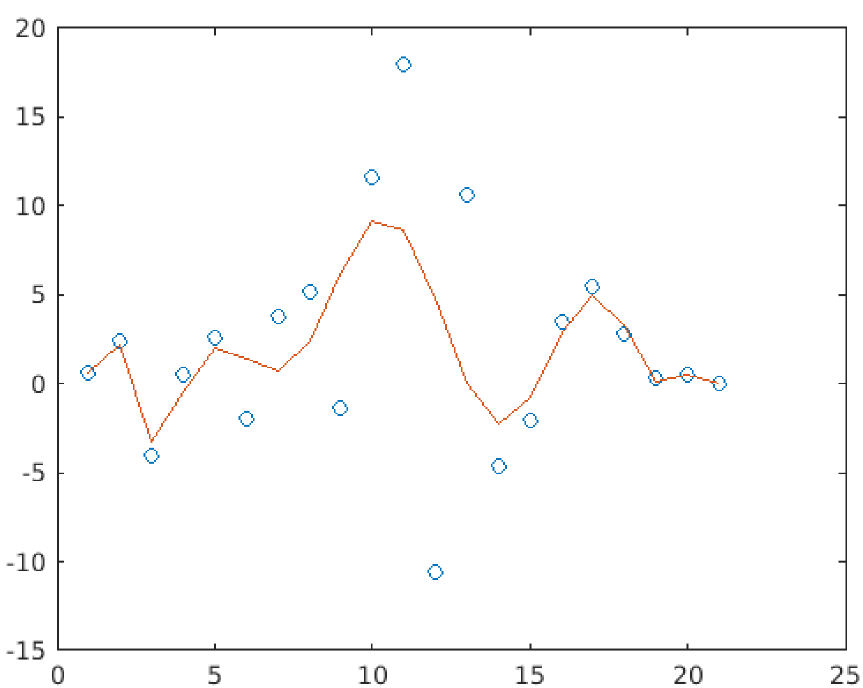


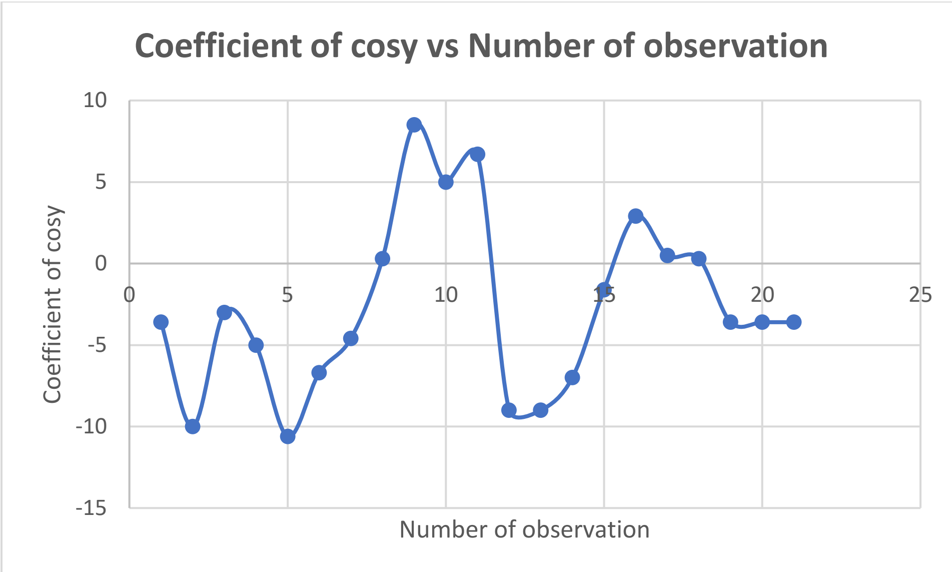


Equation:

$$a_{sin(y)}(t) = 0.1t^9-2t^8 + 42{,}8t^7-606.4t^6 + 56662.2t^5-34466.3t^4 + 132023.5t^3-296928.3t^2 + 342855.7t-147952.6$$

Plot:

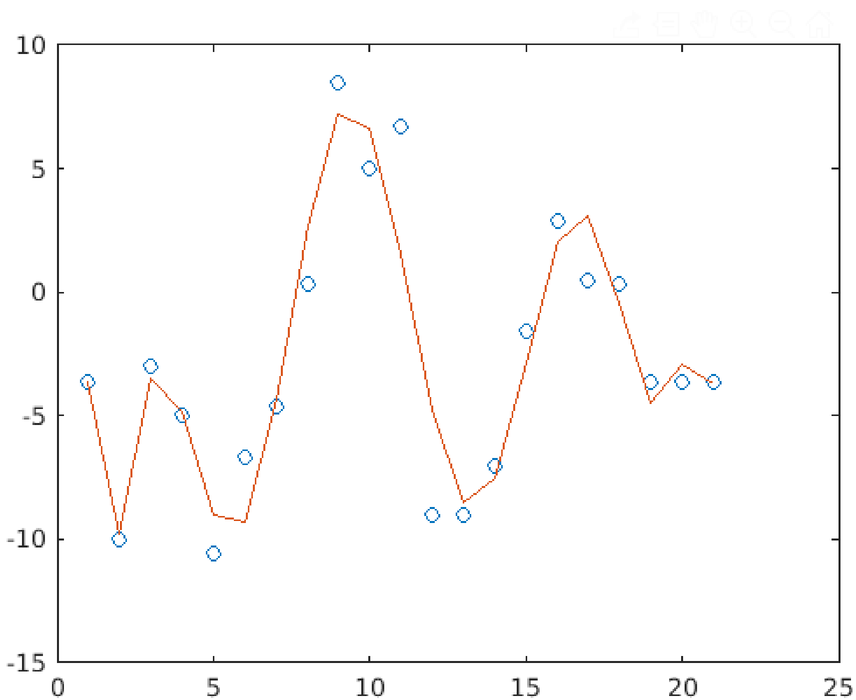


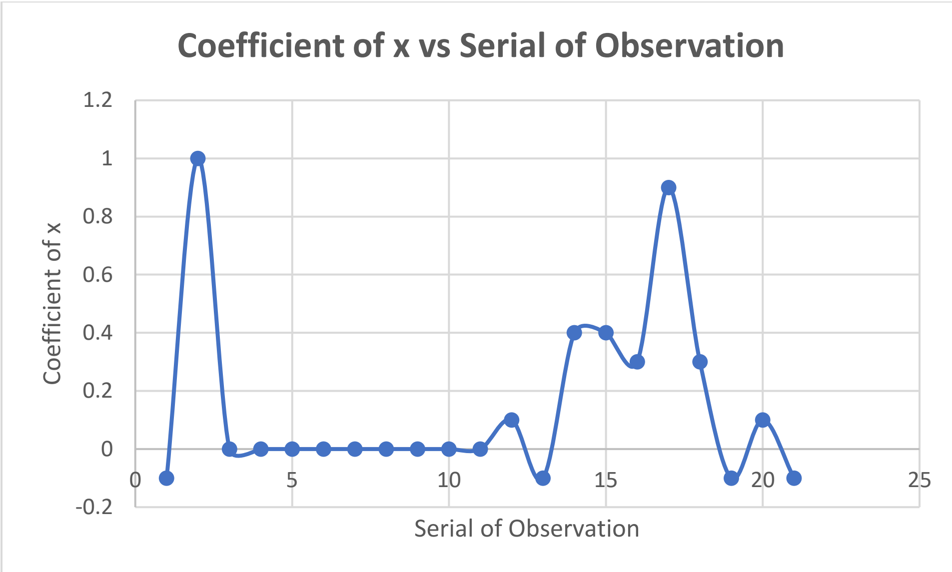


Equation:

$$a_{cos(y)}(t) = 0.0001t^8 - 0.0046t^7 + 0.1059t^6 - 1.4584t^5 + 12.1783t^4 - 60.4108t^3 + 167.7110t^2 - 230.0063t + 108.2569$$

Plot:

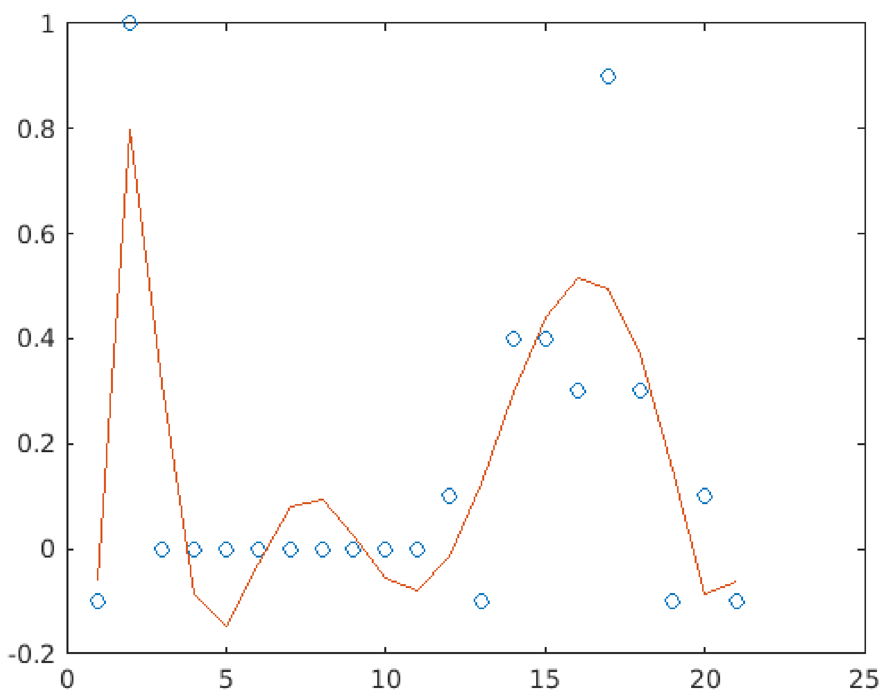


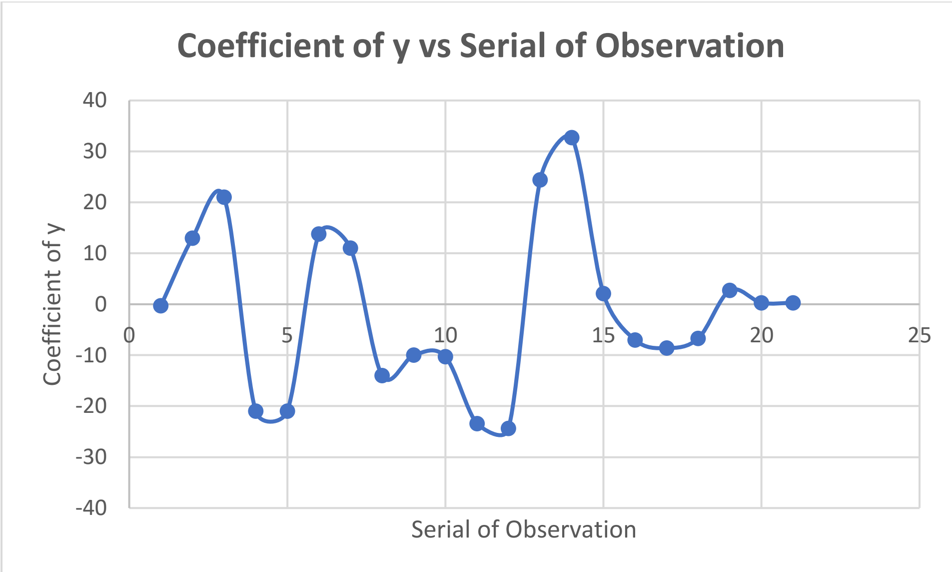


Equation:

$a_x(t) = 0.001t^7 - 0.0020t^6 + 0.0327t^5 - 0.3236t^4 + 1.9446t^3 - 6.6460t^2 + 11.143t - 6.2084$

Plot:

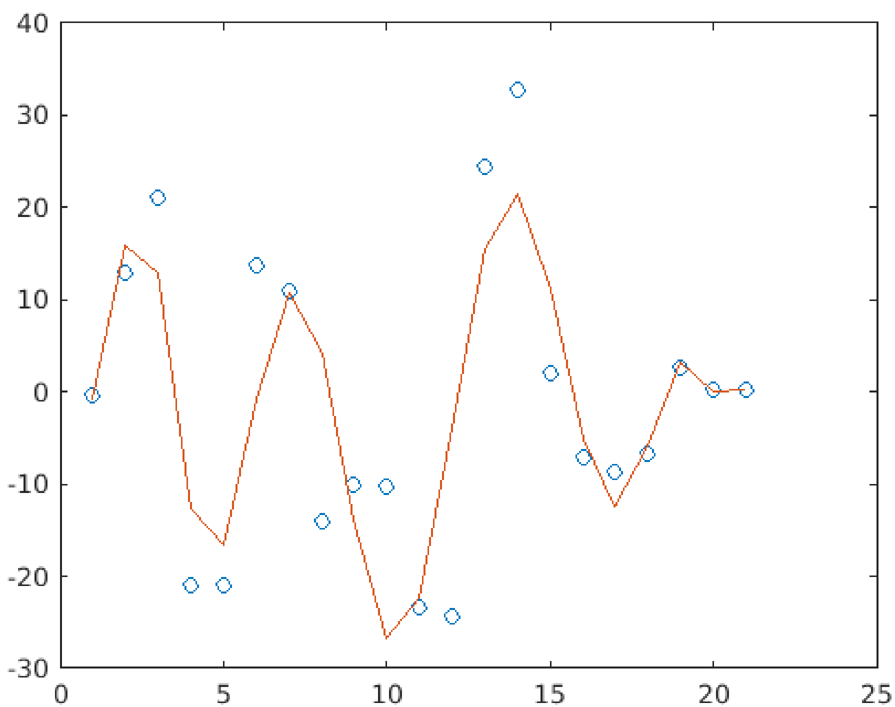


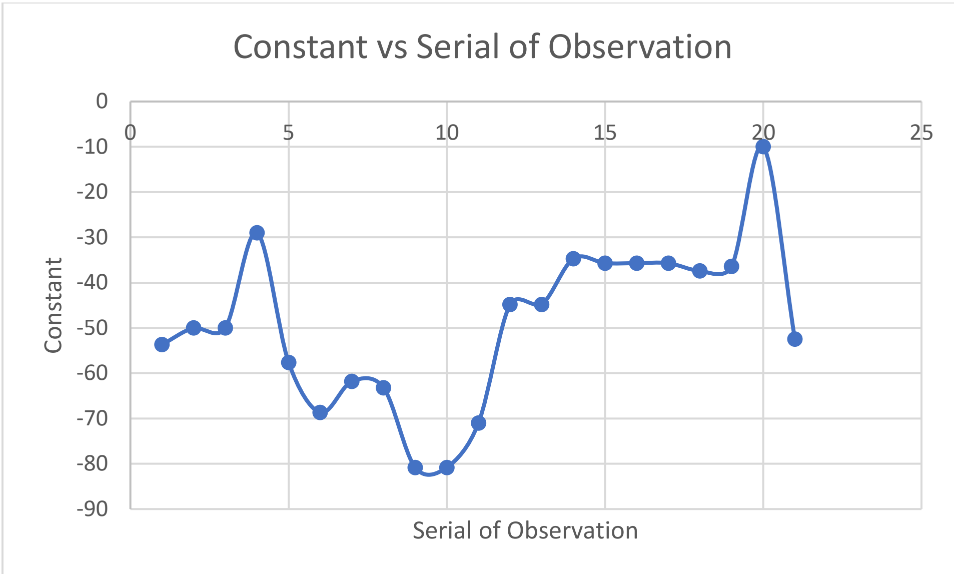


Equation:

$a_y(t)$ = -0.2t^7 + 3.2t^6-28.3t^5 + 159.9t^4-560t^3 + 1128.1t^2-1.1443t + 440

Plot:

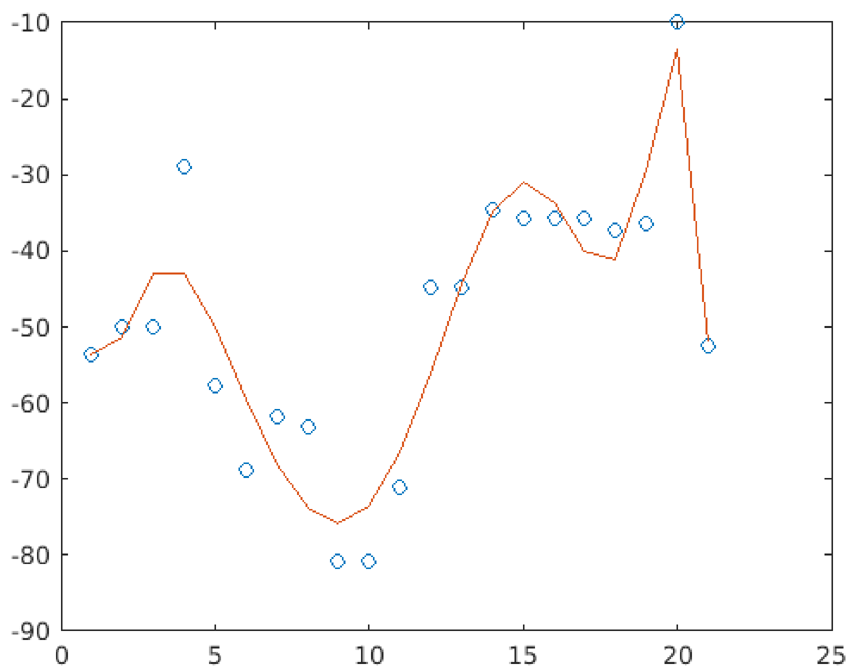




Equation:

$a_{const}(t)$ = 0.0001t^6-0.0029t^6 + 0.0634t^6-0.8375t^5 + 6.9328t^4-35.0729t^3 + 99.0529t^2-130.992t + 7.2007

Plot:



3.2. The effect of each coefficient on the shape of fluid droplet:

Increase of $a_{x^4}(t)$ or $a_{x^2}(t)$ causes contraction of the middle part of the droplet while decrease of it cause expansion in both left and right.

Increase of $a_{y^4}(t)$ or $a_{y^2}(t)$ or $a_{const}(t)$ causes upper part of the droplet coming close to the ground and decrease of it raises the upper portion of the droplet.

Increase of $a_{x^2y^2}(t)$ contracts the upper region of the droplet and decrease of it expands the droplet in both left and right.

Decreasing the value of $a_x(t)$ makes the bottom surface of the droplet tends to move to the right direction and vice versa.

Increasing of $a_y(t)$ indicates that molecules are moving from upper to lower portion through center of mass and vice versa.

Increase of $a_{sin(x)}(t)$ indicates that indicate that upper portion of the droplet is directing to the upper left direction and vice versa.

Increase of $a_{cos(x)}(t)$ means that there is lack central pressure from the top and vice versa.

Increase in $a_{sin(y)}(t)$ expands the center portion in both left and right and decrease of it indicates that there is lack of water molecules and pressure in middle portion.

Increase in $a_{cos(y)}(t)$ indicates that the molecules tend to contract from left and right and they tend to rise up due to the impact of superhydrophobic surface.

IV. Discussion

From the analysis doing above, it can be said that we would be able top track a certain molecule in such droplet. To do this let's again give a look at the above equations. Here we have to consider 1 unit=0.5s in the coefficient vs time graph as we took 21 pictures within 11s. Next, we have to track a certain point in the initial graph comparing it with a molecule. Next, we need to differentiate the equations in section 3.1 to approximate the change of co-efficient during that time. Using the result of 3.2 we can easily find that at which direction of the molecule may tends to go. Then using the formula of molecular dynamics, we would get enough information so that we can track a certain molecule of a droplet. The technology to track a molecule may lead us to track a certain nucleus of a droplet. Finally, it could be developed to navigate the position of a certain nucleus in a large fluid body system. Thus, this concept may pave a new way for early disease detection in blood vessel. This would also play a crucial role in nanotechnology.

Three limitation has been recorded here. First of all this is two dimensional procedure. Three-dimensional approach may take time but it would be more realistic. Secondly, everything has been modeled using 21 images. Use of more images may give more accurate result. Finally, this experiment has been performed on superhydrophobic surface. Different surfaces may give different results and combination of all results could be a breakthrough.

V. Reference

[1] https://www.nature.com/articles/nature15738

[2]https://pdfs.semanticscholar.org/b424/1a8e9497eecd8c49a4bf16d856aaad400402.pdf?_ga=2.122168395.190034826.1603742601-1842470081.1602157072

[3]https://www.youtube.com/watch?v=pzbEMk3_3zo

[4] https://drive.google.com/file/d/1ChSiseK4oGgS0OHPaCAZyNevfTafaYnA/view?usp=sharing