END TERM REPORT

Rohan Virmani, Dr.Rahul Mangal
Department of Chemical Engineering

PROJECT NAME: ACTIVE-COLLOID self-propelled particle motion

TIMELINE: May 14 -July 11-2023

INTRODUCTION

- Active colloids are self-propelled particles that can move through a fluid environment by converting energy from their surroundings into directed motion. They are typically made of microscopic particles that have been coated with different materials on their surface, creating a difference in chemical or physical properties between the two sides. This asymmetry allows the particle to create a local gradient in its surroundings, which drives the particle's motion.

- There are a number of different mechanisms that can be used to create self-propelled motion in active colloids. Some of the most common mechanisms.We have worked with :

- **Diffusiophoresis**: This is the movement of a particle due to a gradient in the concentration of a solute. For example, a particle that is coated with a catalyst that can decompose hydrogen peroxide will create a local gradient in the concentration of oxygen, which will cause the particle to move in the direction of the higher oxygen concentration.

- **Marangoni flow:** Marangoni effect, also known as the Gibbs–Marangoni effect, is the mass transfer along an interface between two phases due to a gradient of the surface tension. Can be caused by a variety of factors like SURFACTANTS.

References: Dynamics of active SiO2-Pt Janus Colloids in dilute Poly(EthyleneOxide) solutions, ACS Physical Chemistry Au 2023
Acknowledgements: Department of Chemical Engineering, IIT Kanpur and Centre for Continuing Education, IIT Kanpur

Application no. - 2330313
Applicant - Rohan Virmani
Mentor - Dr. Rahul Mangal
Department of Chemical Engineering, IIT Kanpur

ABSTRACT

- The collective motion refers to the coordinated movement exhibited by a group of droplets or particles that are self-propelled. These can exhibit intriguing behaviors similar to living organisms, despite lacking a centralized control mechanism. This phenomenon is typically observed in systems where they are chemically or physically active, generating internal energy that drives their motion.

- There are a number of different mechanisms that can lead to collective motion. In some cases, the interaction between the agents is purely physical. For example, in a system of droplets that are moving on a surface, the droplets can interact with each other through surface tension. This interaction can lead to the formation of patterns, such as spirals or vortices.

- The study of collective motion is a rapidly growing field, and there is a great deal that we do not yet understand about it. However, it is a fascinating and important phenomenon, with a wide range of potential applications like:

- Colonies of bacteria: Colonies of bacteria are able to form coordinated structures, such as biofilms. These structures can help the bacteria to survive in their environment.

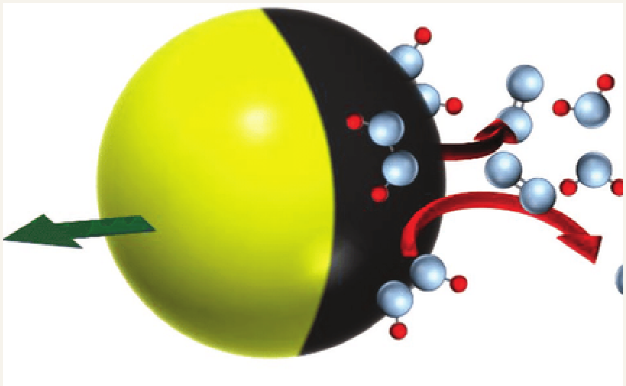
- Targeted Drug delivery: Self-diffusiophoretic particles can be used to deliver drugs to specific locations in the body. For example, a particle that is coated with a ligand that binds to a specific receptor on a cell can be used to deliver a drug to that cell.

SYSTEM I

Hybrid particles consisting of a silica (SiO2) core and a platinum (Pt) shell, exhibiting distinct properties on each side. Allowing unique functionalities and applications due to the different surface properties and chemical reactivity of the two sides.

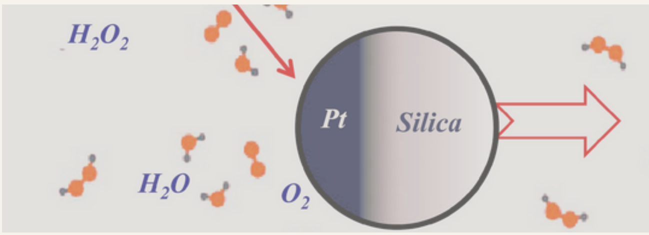
SYSTEM USED IN STUDY-5um Janus colloid +1%wtH2O2

A Janus particle is a microscopic particle with two distinct physical properties. This unique surface of Janus particles allows two different types of chemistry to occur on the same particle. The simplest case of a Janus particle is achieved by dividing the particle into two distinct parts, each of them either made of a different material, or bearing different functional groups.



$$H_2O_2 \xrightarrow{Pt} H_2O + \frac{1}{2} O_2$$

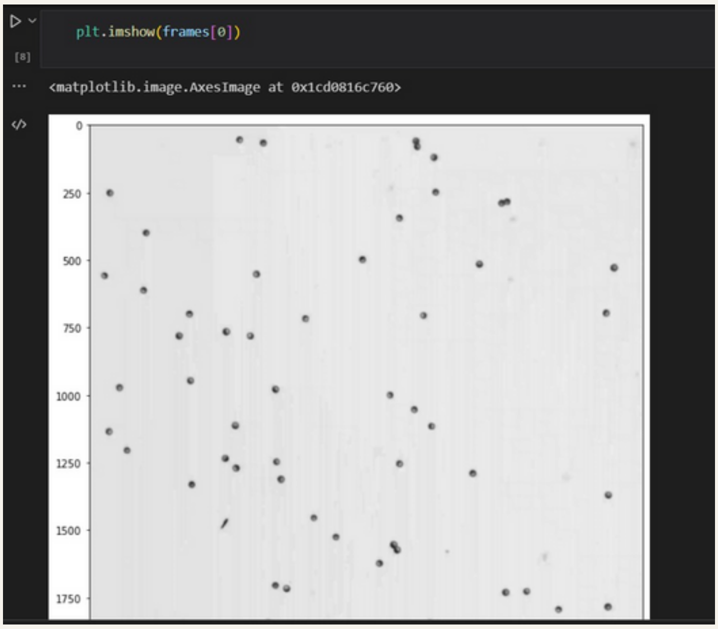
This setting works on the principle of **SELF-DIFFUSIOPHORESIS .** The O2 concentration increases on the platinum side and so the water concentration decreases on the SiO2 and so the solvent moves from low to high concentration and so to maintain the momentum balance the particle moves in the opposite direction , that is the sillica side .



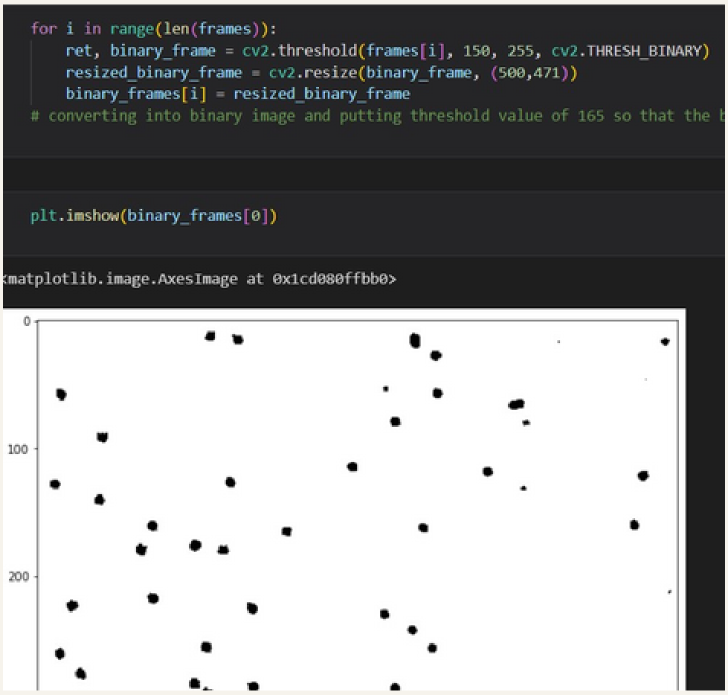
Self-diffusiophoresis occurs when a particle has a surface that is chemically or physically asymmetric. This asymmetry creates a difference in the rate at which the solute diffuses to the two sides of the particle. This difference in the rate of diffusion creates a gradient in the concentration of the solute, which in turn creates a force on the particle. The direction of the force depends on the direction of the concentration gradient.

WORKING

The system was observed and videos were worked upon through IMAGEJ, Spin-view and tools like open-cv and trackpy.



The full video was divided in a list of frames starting from '0'. The Frame is resized to get maximum no of particles with clear motion. This video had a total of 85 particles in all .

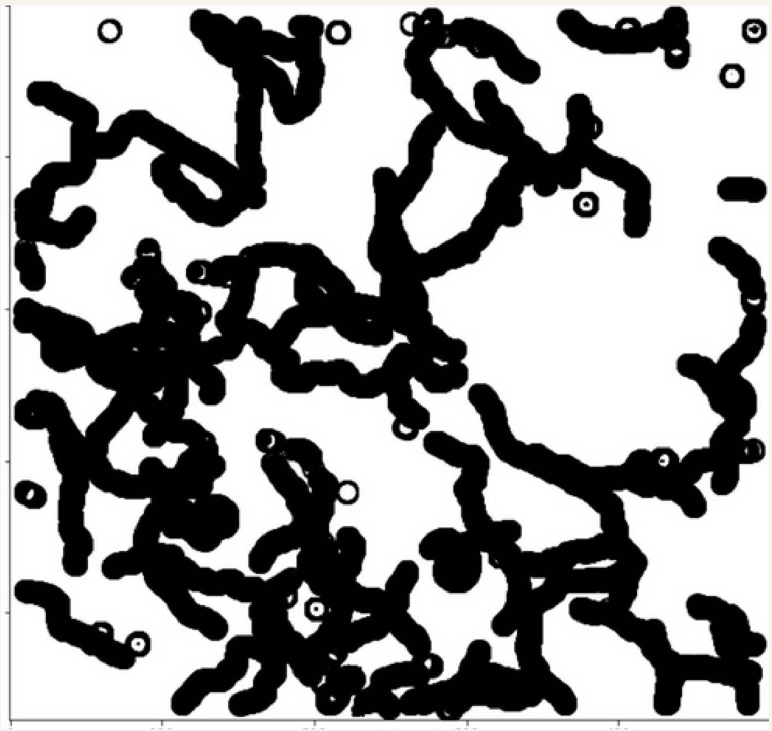


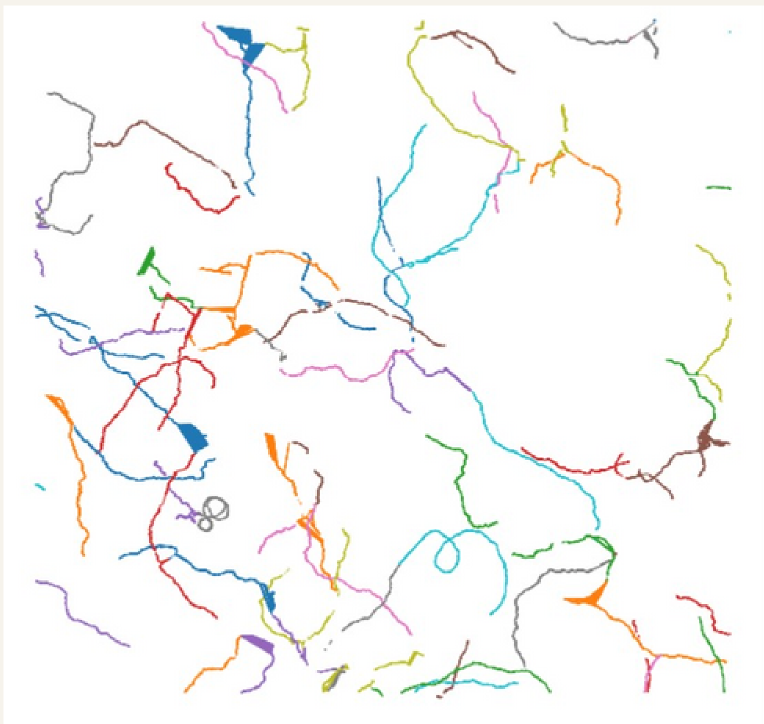
The frames were converted into a binary frame(Black and White) using an appropriate threshold value as a limit so that the trajectories can be tracked easily with the help of center of mass . OPEN-CV library was used in python to get the required result .

The TrackPy batch algorithm was used to get frame wise data of various particles giving some of the parameters as shown.

	y	x	mass	size	ecc	signal	raw_mass	ep	frame
0	14.748872	156.120576	10699.933590	3.059453	0.103989	229.257772	-82309.0	0.0	0
1	27.292800	310.773582	11060.063208	3.048107	0.065436	227.401434	-81598.0	0.0	0
2	53.510217	271.794754	3043.466537	1.958708	0.030890	209.766221	-92319.0	0.0	0
3	56.825123	312.035862	9627.898259	2.830880	0.037708	232.042279	-83893.0	0.0	0
4	57.684807	18.171138	10966.318127	3.091440	0.112811	228.329603	-81949.0	0.0	0
5	65.533159	373.837732	14877.622789	3.815837	0.300665	216.263404	-75549.0	0.0	0
6	79.023488	279.215928	9405.137671	2.806606	0.047989	232.042279	-84217.0	0.0	0
7	91.144027	50.494500	10884.639244	3.083154	0.077339	228.329603	-82080.0	0.0	0
8	114.243049	245.788113	9948.116605	2.897483	0.076025	231.114110	-83446.0	0.0	0
9	118.124469	351.332101	10044.646193	2.902388	0.063524	231.114110	-83316.0	0.0	0
10	121.324207	472.819699	11119.466031	3.049371	0.062563	228.329603	-81767.0	0.0	0

All the frames were annotated , that is kind of overlayed and the trajectories were somewhat made visible (of different particles)

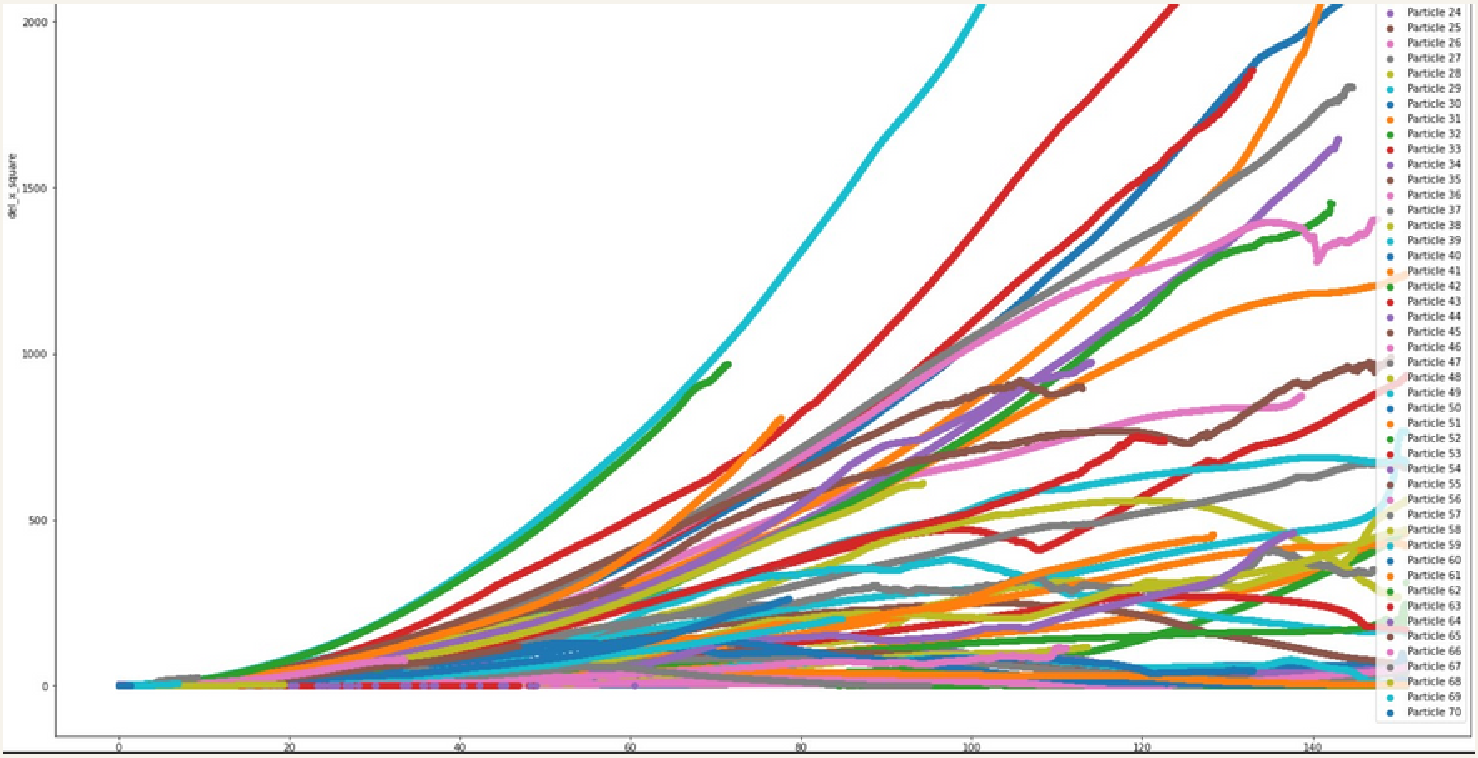




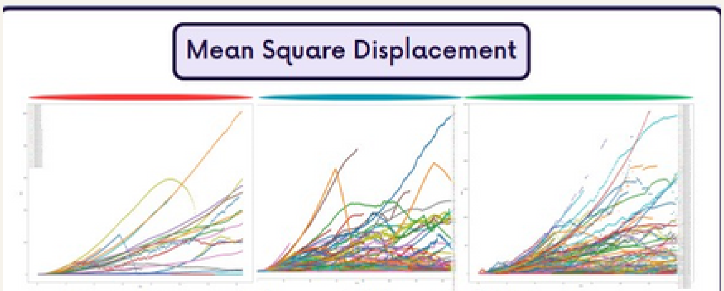
But to get the trajectories in a mathematical form we will the X and Y coordinate of the particle and also the angle of orientation . In order to maybe further predict the position an d study the collective motion better.

frame	particle	...	dx	dy	dr	vx	vy	s	sma	avrad	avdeg	avdeg1
0	0	...	0.397113	0.290045	0.961563	0.794226	0.580091	1.923125	21.331228	0.630829	36.143835	36.143835
1	0	...	-9.208478	-0.844869	-21.016174	-18.416956	-1.689738	42.032348	21.163227	-3.050100	-174.757843	-174.757843
2	0	...	-9.039561	-0.893036	-20.644278	-18.079121	-1.786071	41.288557	21.370491	-3.043120	-174.357946	-174.357946
3	0	...	-9.174379	-0.945628	-20.960618	-18.348757	-1.891256	41.921236	21.600040	-3.038883	-174.115150	-174.115150
4	0	...	-9.251248	-1.177993	-21.185478	-18.502495	-2.355987	42.370956	21.766314	-3.014941	-172.743382	-172.743382
...	...	...	...	...	...	...	...	...	...	...	...	...
3014	84	...	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
3015	84	...	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
3016	84	...	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
3017	84	...	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
3018	84	...	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

SOME RESULTS



The Mean Square displacement was also plotted particle wise .This was tested for increasing number of particles .



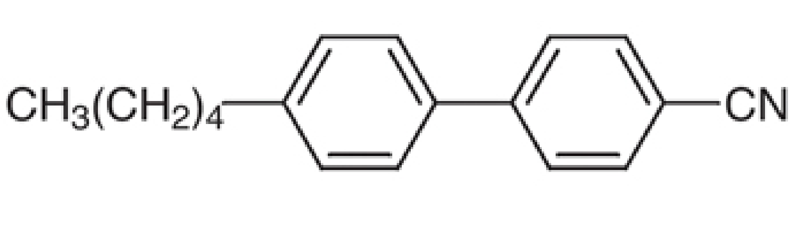
Observed increase in the speed of the peak of M.S.D. vs time curve correlates with the growing number of particles

SYSTEM II

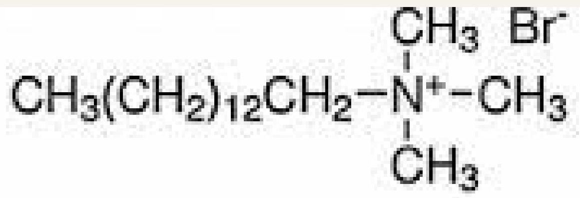
SYSTEM USED IN STUDY-5um Janus colloid +1%wtH2O2

5CB-Liquid Crystal droplets -TTAB (aq) solution

5CB (4-cyano-4'-pentylbiphenyl) is a commonly used liquid crystal compound which is working an oil droplet here.



TTAB or ,Tetradecyltrimethylammonium bromide. is a cationic surfactant which provides stability of oil droplets in water.



Tetradecyltrimethylammonium bromide (TTAB)

The collective motion in this case is fueled by the MARANGONI FLOW MECHANISM. Marangoni flow self-propulsion is a mechanism by which a particle can move through a fluid by creating a difference in surface tension. This difference in surface tension creates a flow of fluid, which propels the particle .

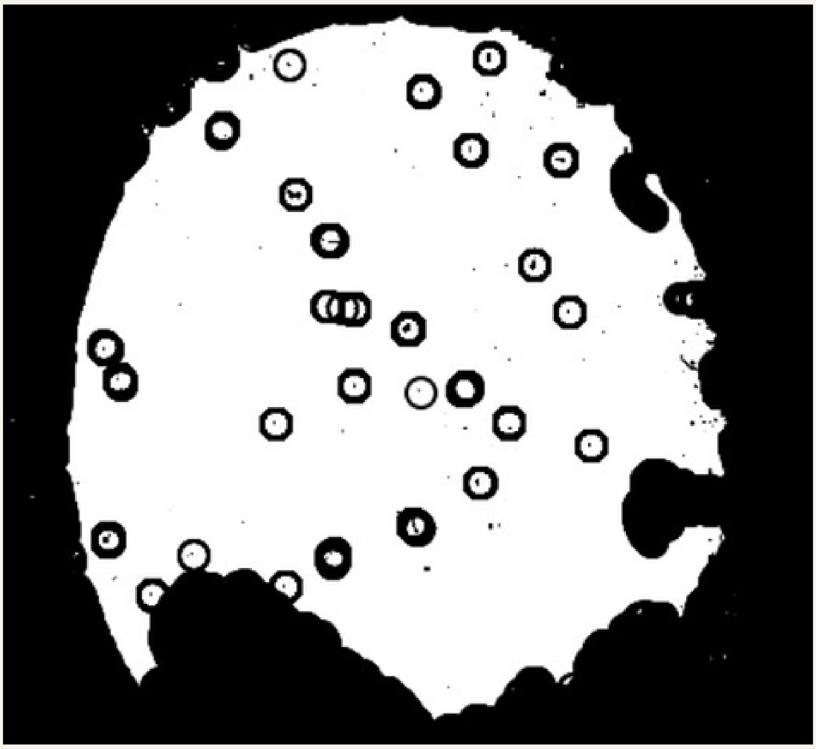
- It is a sensitive mechanism, which means that it can be affected by changes in the environment.

SETTING -

Water , 6%wt TTAB With 300 droplets of 5CB (70-80 um)

{1wt%PEO}(poly-ethyleneoxide) , 6%wt TTAB With 300-350 droplets of 5CB (70-80 um)

A HELE-SHAW cell was created by creating a well of 10x7 mm of double sided tape with a thickness of 100um. TTAB solution was put on the cover slide with a pipette. The droplets of 5CB were put by a MICRO-INJECTOR .The droplet size is about 70-80 um and is first checked before adding 300 of those inside the solution on the cover slip.



Helped in preparation of the Hele-Shaw cell of 10*7 mm with a 100 m thick double sided tape and sealed with nailpaint to avoid convection.
Got to work out basics of an upright microscope. And learnt about Fluorescent microscopy. Again use the TrackPy and open-cv on the spinview recorded videos to binary particle videos for particle wise analysis.

mass	size	frame	particle
13043.225868	6.705206	0	0
12585.248941	6.522784	1	0
12818.843166	6.531152	2	0
12136.547657	6.584243	3	0
12613.466470	6.633354	4	0
...	...	...	...
12686.020852	6.505836	4018	0
12853.292332	6.511824	4019	0
12956.249409	6.485217	4020	0
12255.523991	6.399207	4022	0
12385.320128	6.624398	4023	0

Analysis of single particle showed continuous decrease in the size pointing to some SOLUBILISATION whose rate can be calculated in the terms of decrease in radius per unit time .

This work was just started in the last week . This decrease in size in because of the solubilisation of the some small part of the oil drop into the empty micelle of TTAB.