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STUDY OF SANS DISTRIBUTION FUNCTION FOR DIFFERENT PARTICLES AT DIFFERENT CONDITIONS

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ABSTRACT

The size and shape of a particle can be found out by the analysis of form factor distributions in small angle neutron scattering. In the present work, the form factors were calculated theoretically by computer program and their plots were analyzed to find out the size and shape of the particles. The structure factor, on the other hand was found to be very useful to find out the particle separation and concentration of the particles. The structure factors were calculated for three potentials (i) Screened Coulomb Potential (ii) Hard Sphere Repulsion and (iii) Baxter Hard Sphere Model and their plots were analyzed to see the effects of structure factor on particle separation, concentration, particle charge, potential height, potential width and temperature.

Key words: SANS, Form factor, Structure factor, Contrast factor.

I. INTRODUCTION

Small angle neutron scattering (SANS) is relatively a new member of neutron scattering techniques [1] in which a beam of thermal neutron is scattered by particles dispersed in a solvent or matrix in the length scale of 10 to 1000Å [2] provided that the scattering length density of solvent and the particles are different so that the combination can form high contrast factor. SANS uses the thermal neutrons whose average velocity is nearly 2200ms^{-1} and the corresponding de-Broglie wavelength is 1.8Å and energy 25meV [3].

The differential cross-section $\frac{d\Sigma}{d\Omega}$ of SANS can be expressed in terms of two factors, denoted by form factor P(Q) and structure factor S(Q). The form factor P(Q) depends on the size and shape of the particles and the structure factor S(Q) depends on the interaction potential between the particles. The study of the shapes of the curves of P(Q) and S(Q) over Q gives the idea of the size and shape of the particles and the kind of interaction that exists among the particles. Here Q is the wave vector transfer in the scattering process.

II. METHODOLOGY

The form factors and the structure factors for different types of particles and for different interaction potential are calculated by the computer program “PQ.for” and “SQ.for”. The theoretically derived data are plotted to observe the shapes of their curves. By applying different approximations to the form factor curves, the presumed values of the dimension of the particles are recalculated and compared with their actual values. The structure factor curves for three potentials known as i) Screened Coulomb Interaction ii) Hard Sphere Repulsion & iii) Baxter Hard Sphere Model, were studied to observe variations with radius, charge, concentration and temperature of the particles.

III. THEORY

3.1 The Form Factors:

For spherical particle of radius R, the form factor P(Q) first derived by Rayleigh (1914) is

$$P(Q)=[\frac{3sinQR-QRcosQR}{(QR)^3}] \quad \text{------------ (1)}$$

The function has a central maximum at Q=0 followed by a series of maxima and minima.

For cylindrical or disk type particles of diameter 2R and height 2*l*, P(Q) is written as

$$P(Q)=\int\frac{sin(Qlcos\beta)4J_1^2(QRsin\beta)}{Q^2l^2cos\beta Q^2R^2sin^2\beta}sin\beta d\beta \quad \text{-- (2)}$$

where β is the angle between the axis of the cylinder and bisectrix. J_1 is the Bessel function of order unity, the disk being a special case of cylinder when $l<<R$.

For ellipsoidal particle of major axis 2a and minor axis 2b=2c, the form factor is

$$P(Q)=\int_0^1[F(Q,\mu)]^2d\mu \quad \text{---------------------- (3)}$$

where $F(Q,\mu)=3(sinx-xcosx)/x^3$ and $x=Q[a^2\mu^2+b^2(1-\mu^2)]^{1/2}$, μ is the cosine of the angle between the directions of major axis and the wave vector transfer Q.

3.2 The Guinier Approximation

In the limit Q~0 ($QR_g<1$), the form factor for spherical particle [4] can be approximated to

$$P(Q)=exp(-\frac{Q^2R_g{}^2}{5}) \quad \text{---------------------- (4)}$$

Thus the radius of the particle can be found out from the slope of LnP(Q) Vs Q^2 curve at low Q range with $R_s=\sqrt{(3/5)}R_g$.

For cylindrical particles within the limit $Ql>>1>QR$, P(Q) decreases exponentially as

$$P(Q)=\frac{\pi}{2Ql}exp(-\frac{Q^2R^2}{4}) \quad \text{------------------ (5)}$$

For disk type particles within the limit $Ql<1<<QR$, P(Q) also decreases exponentially as

$$P(Q)=\frac{2}{Q^2R^2}exp(-\frac{Q^2l^2}{3}) \quad \text{--------------- (6)}$$

where $L=2l$ the height for cylindrical and disk particles.

Thus the radius of the cylindrical particle can be found out from the slope of Ln(P(Q)*Q) Vs Q^2 curve and the height of the disk particles can be found out from the slope of Ln(P(Q)*Q) Vs Q curve at low Q range.

3.3 The Structure Factor:

The inter particle structure factor S(Q) is significant when the particles are interacting each other [2, 5, 6, 7]. The interaction depends on the density, radius, charge, temperature etc. The structure factor S(Q) for the isotropic system is given by

$$S(Q)=1+4\pi n\int(g(r)-1)\frac{SinQr}{Qr}r^2dr \quad \text{-- (7)}$$

where g(r) is the radial distribution function, and g(r) is the probability of finding another particle at a distance r from a reference centered at the origin. The details of g(r) depend on the interacting potential between the particles. S(Q) is calculated for the three potentials mentioned before [8,9].

IV. ANALYSIS OF THEORETICAL DATA

(1) The form factors for different sizes of the particles are calculated by computer program “PQ.for” and are plotted as wave vector transfer along the abscissa and the form factors along the ordinate.
(2) Guinier Approximation is applied to the form factor curves and the dimensions of the particles are recalculated.
(3) The structure factors for the three different potentials are calculated by computer program “SQ.for” and are plotted as wave vector

transfer as the abscissa and the form factors as the ordinate.

(4) Form factors and structure factors and their variation with different parameters are studied carefully.

V. FORM FACTOR CURVES OF DIFFERENT TYPES OF PARTICLES

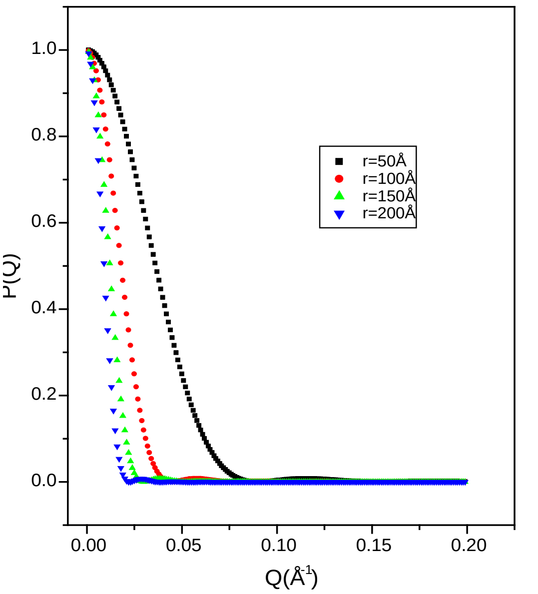

Figure 1: Form factor for spherical type particles for differe

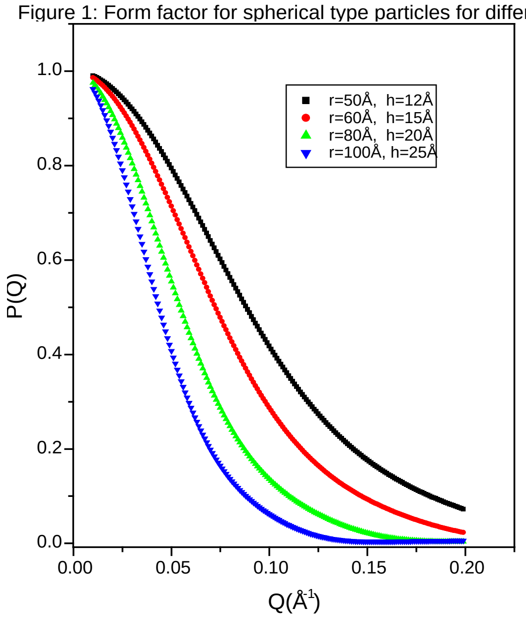

Figure:2 P(Q) Vs Q for cylindrical type particles at different radii and

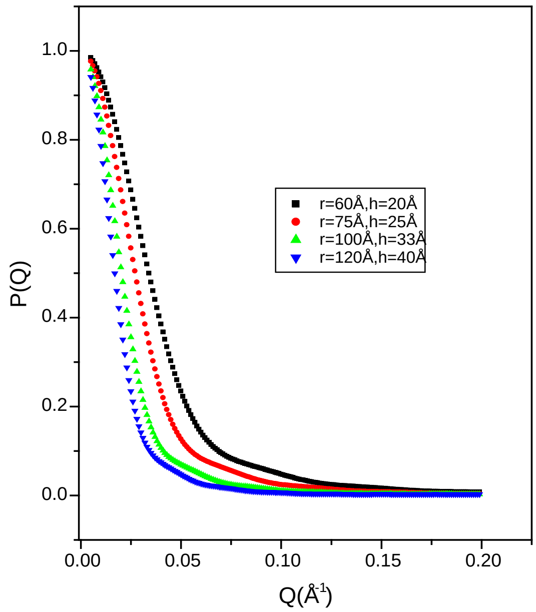

Figure 3: Form factor for disc type particles of different and heights

VI. GUINIER PLOT ANALYSIS

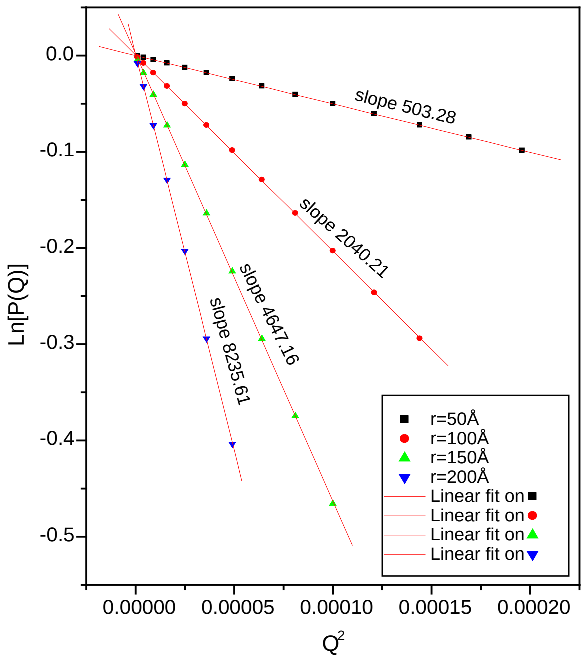

Figure 4: Guinier plot of spherical type particle:

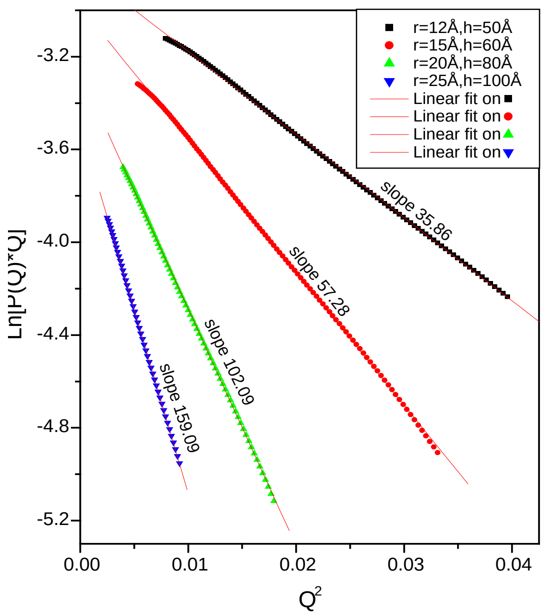

Figure 5: Guinier plot of cylindrical type particles

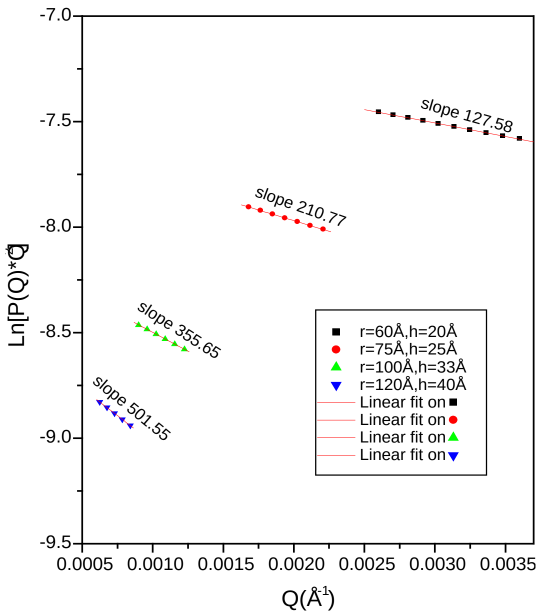

Figure:6 Guinier plot of disc type particles

Table 1: The Guinier plot analysis for spherical particles

Presumed value	Radius R	50 Å	100 Å	150 Å	200 Å
Guinier Analysis	Radius of gyration R_g	38. 86 Å	78.23 Å	118.07 Å	157.18 Å
	Radius of the sphere R_s	50. 12 Å	100.92 Å	152.31 Å	202.77 Å

Table 2: The Guinier plot analysis for cylindrical particles

Presumed value	Radius R	12 Å	15 Å	20 Å	25 Å
	Height L	50 Å	60 Å	80 Å	100 Å
Guinier Analysis	Radius R	11.97 Å	15.13 Å	20.21 Å	25.23 Å

Table 3: The Guinier plot analysis for disk particles

Presumed value	Radius R	60 Å	75 Å	100 Å	120 Å
	Height L	20 Å	25 Å	33 Å	40 Å
Guinier Analysis	Height L	19.56 Å	24.60 Å	32.66 Å	39.31 Å

VII. STRUCTURE FACTOR CURVES FOR DIFFERENT TYPES OF INTERACTIONS

i) Screened Coulomb Interaction

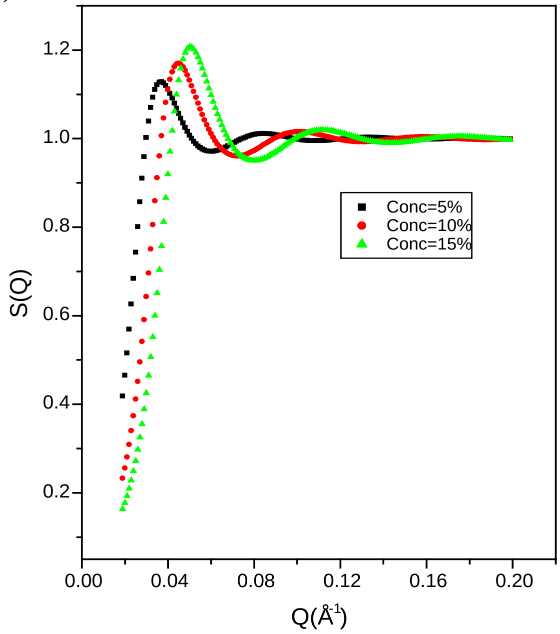

Figure 7: S(Q) Vs Q for different concentrations (Screened C
Interaction) with Const radius(50Å),Charge(15esu),Temp(30

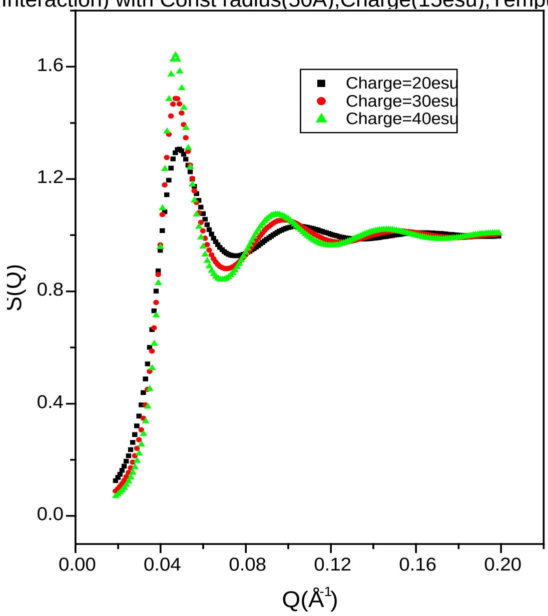

Figure 8: S(Q) Vs. Q for different Charges (Screened Co
Interaction),with constant radius(50Å),Conc.(15%),Temp(

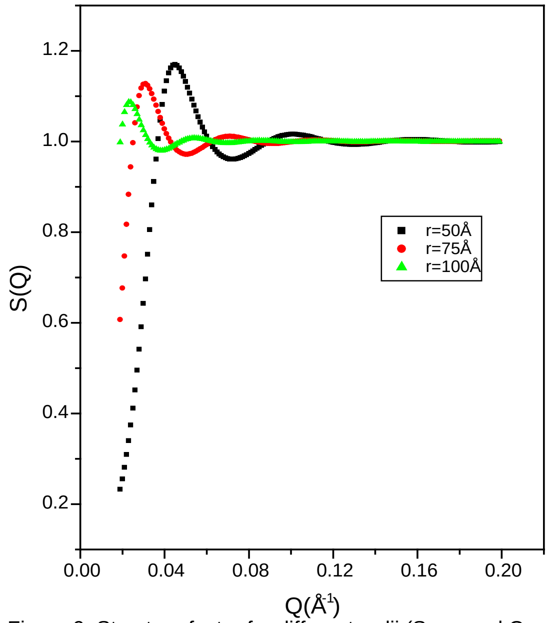

Figure 9: Structure factor for different radii (Screened Cou
Interaction) at constsnt parameters [conc(10%), charge(1
Temp(300K)]

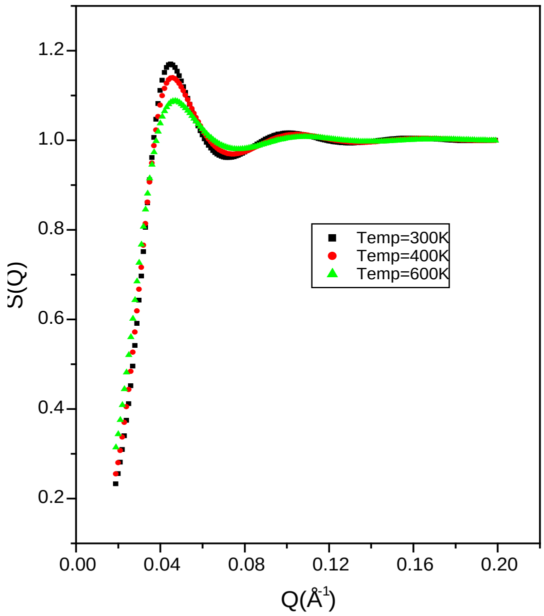

Figure 10: S(Q) Vs Q at different Temperatures (Screened C
Interaction) with constant conc.(10%),radius(50Å),charge(15

ii) Structure factor for Hard Sphere Repulsion

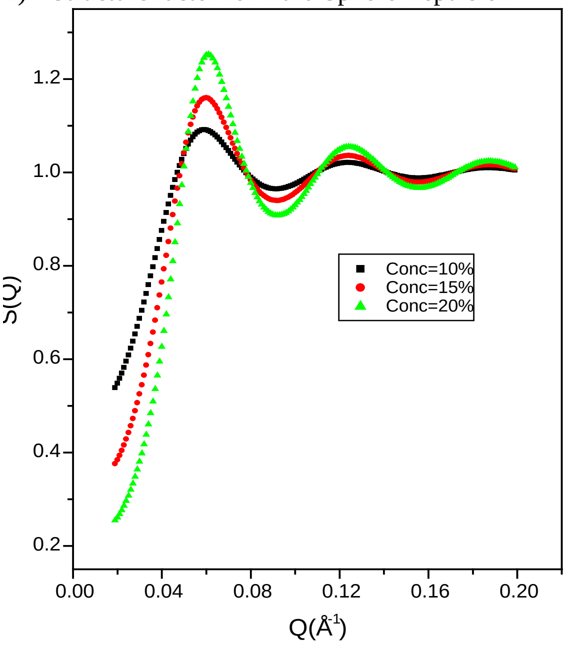

Figure 11: S(Q) Vs Q for different concentrations (Hard S
Repulsion)with constant radius(50Å),Temp(300).

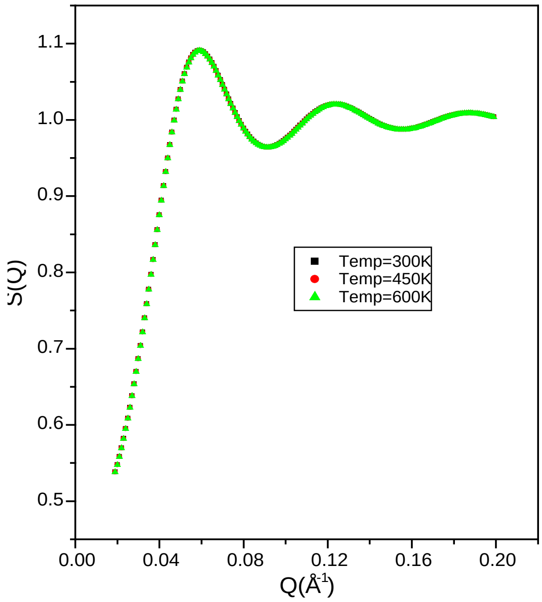

Figure 13: S(Q) Vs Q at different temperatures (Hard S
Repulsion) and with constant radius(50Å),conc.(10%).

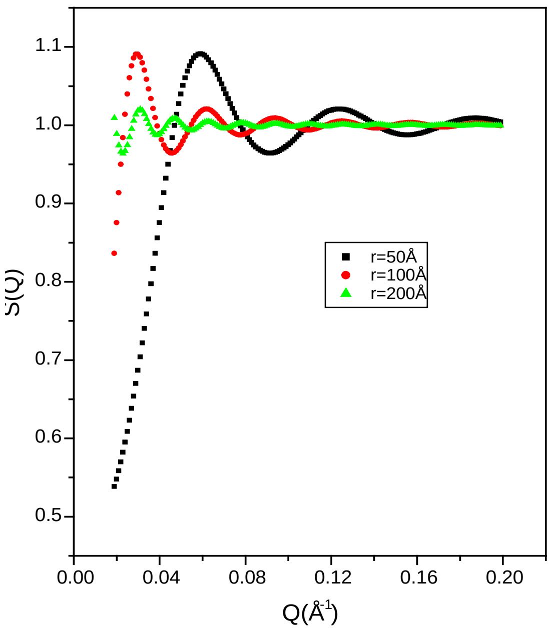

Figure 12: Structure factor for different radii (Hard Sphere Rep
Constant parameters conc(10%),Temp(300K),

iii) Structure factor for Baxter Hard Sphere Model

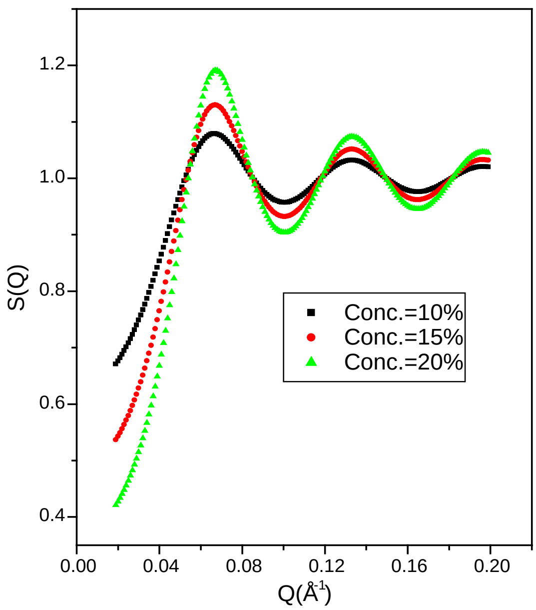

Fig14: S(Q) Vs Q for different concentrations (Baxter Hard Sphere M
with constant radious(50A),Temp.(300K),Potential width(2A) & Heig

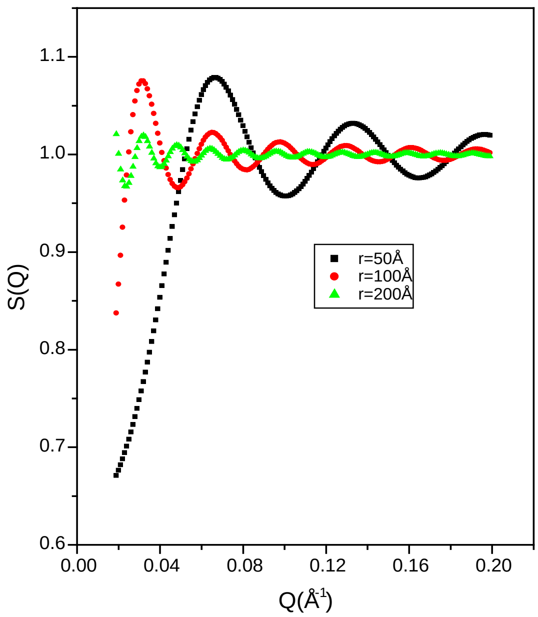

Figure 15: S(Q) Vs Q for different radii (Baxter Hard Sphere Model) with constant conc.(10%),Temp.(300K),potential width(2A) and hei$_B$T)

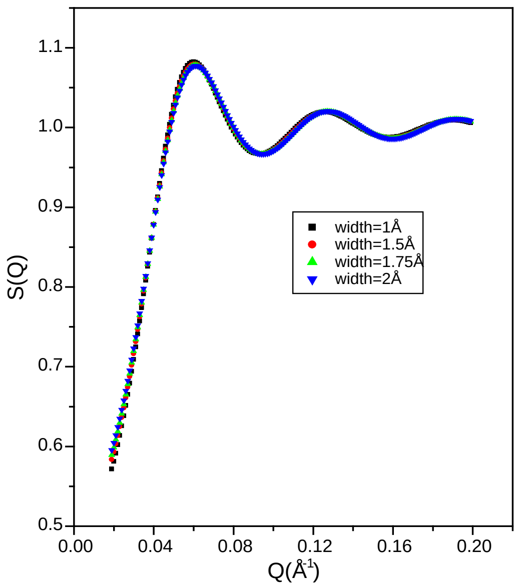

Figure 17: S(Q) Vs Q for different Potential width(Baxter Hard Sphere with constant potential height($_B$T),radius(50Å),Temp.(300K),conc.(10%

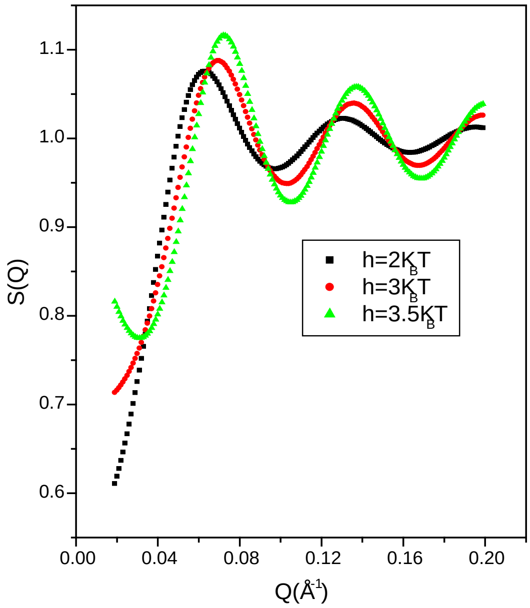

Fig 16: S(Q) Vs Q with varying potential height (Baxter Hard Sphere at constant potential width(1Å),radius(50Å),Temp.(300K),Conc.(10%

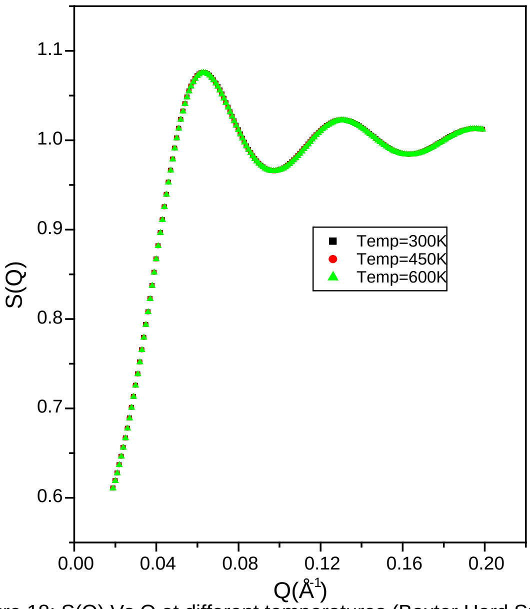

Figure 18: S(Q) Vs Q at different temperatures (Baxter Hard Sphere with constant radius(50Å),conc.(10%),Potential width(1Å) and hei$_B$T)

VIII. RESULTS AND DISCUSSION

Form Factor distribution: The form factor curves have the definite shapes for definite dimensions of the particles. Figure 1 shows the form factor for spherical particles for different radii. The form factor for spherical particles decreases from a maximum value and sharply it becomes flat with a series of maxima and minima. Figure 2 shows the form factor for cylindrical particles for different radii and height. The values are decreasing with Q value without any sharp changes. Figure 3 shows the form factor for disk type particles for different radii and height. The form factor decreases for disk type particles and becomes flat with larger Q value with a continuous change in the middle. Further, for all shapes, as the size of the particle is greater, we see a narrower distribution. On the other hand the Guinier plot analysis of the form factor curves gives the measurement of the dimension of the particles with high accuracy. The figure 4 indicates the Guinier plot analysis at low Q region for spherical type particles. Figure 5 indicates the Guinier plot analysis at low Q region for cylindrical type particles. Figure 6 indicates the Guinier plot analysis at low Q region for disk type particles. All the results of Guinier plot analysis are summarized in the tables 1, 2 and 3 respectively.

Structure factor distribution: The structure factor curves give the information about how structure factor varies with the particle dimensions, concentrations, charges, temperatures, potential width and height etc for three afore-mentioned potentials. S(Q) shows maxima and minima of decreasing amplitude. The first peak always occurs at $2\pi/d$, where d is the inter particle separation. **i) Screened Coulomb Interaction:** The effect of concentration on S(Q) for screened coulomb interaction is shown in Figure 7. As the concentration of the particles increases, the inter particle separation decreases with increasing coulomb interaction and S(Q) reaches its higher value and also shifts to the higher Q value. The effect of particle charge on S(Q) is shown in Figure 8. As the charge of the particle increases, the effect of the electrostatic interaction increases between the particles. As a result the distance between the particles increases and the peak value of S(Q) rises to its higher value. The peak of S(Q) also broadens with the decrease in charge as a result of the reduction in the Coulomb interaction between the particles. Figure 9 shows the effect of particle radius on S(Q). A smaller value of the radius of the particle increases stronger coulomb interaction between the particles and the peak increases to its higher value. The distance between the particles becomes less and peak also shifts to higher Q values. It is important to note here that as the particles become larger, S(Q) tends to unity, i.e. the coulomb interaction becomes negligible. Figure 10 shows the effect of particle temperature on S(Q). No remarkable change is observed with temperature **ii) Hard Sphere Repulsion:** The effect of concentration on S(Q) for Hard Sphere Repulsion is shown in Figure 11. As the concentration is decreased, the peak of the S(Q) curve broadens without significant shift of the peak position. The peak becomes broad as a result of the reduction of the interaction between the particles. As the concentration of the particle increases, it is also found that the peak value increases by a significant amount. The effect of particle radius on S(Q) is shown in Figure 12. Smaller the radius of the particle higher is the interaction between the particles. The distance between the particles become less and peak shifts to higher Q values. Figure 13 shows the effect of temperature on S(Q) which is found to be independent with variation of particle temperature. **iii) Baxter Hard Sphere Model:** The effect of particle concentration on S(Q) for Baxter Hard Sphere Model is shown in Figure 14. As the concentration is decreased, the peak broadens without significant shifting of the peak position with Q value. The broadening of the peak takes place as a result of the reduction in the interaction between the particles. The effect of particle radius on S(Q) is shown in Figure 15. Smaller the radius of the particle higher is the interaction between the particles. The distance between the particles become less and peak shifts to higher Q values. The broadening and diminishing of the peak with the increase of radius is due to weak interaction between the particles. The effect of different potential width and height on S(Q) is shown in Figure 16 and Figure 17. It is important to note that no significant changes in S(Q) have occurred by changing the potential width, further, which has occurred in the case of changing the potential height. As the potential height takes the larger value, the peak value on S(Q) increases and shifts to the higher Q values. The effect of particle temperature on S(Q) is shown in Figure 18. It is remarked that no significant variation occurs as the temperature changes.

IX. CONCLUSION

SANS gives a good result if the contrast factor of the solvent with the particles is high. So the selection of solvent should be made for which the contrast factor attains a higher value. The evaluated parameters of the particles from the form factor curves are compared with their presumed values and agrees with a good accordance. The structure factor curves indicate the variations of its value with the concentration, charge, radius, temperature, potential height and width etc. Therefore any experimental curve analysis in this manner identifies the size and shape of the particles and the kind of interaction that exists among the particles.

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