This document recommends some SANS data fitting models, available in fitting packages at ISIS, for inclusion in SANSView.

The names in brackets in the "Model" field are the subroutine name (eg, Debye), and the FORTRAN module name (eg, DEBYE.FOR).

Variables:

| | |
|---|---|
| $B$ | Background |
| $I$ | Cross-section |
| $Q$ | Scattering vector |
| $N$ | Number density of scatterers |
| $V$ | Volume of a scatterer |
| $\phi_p$ | Volume fraction of particles |
| $\rho$ | Scattering length density |
| $\delta$ | Bulk density of scatterer |
| $N_{agg}$ | Cluster aggregation number |
| $R_p$ / $R$ / $R_0$ | Particle (spherical) radius |
| $R_g$ / $r_g$ | Radius-of-gyration |
| $\sigma$ | Second moment of distribution (layer thickness) |
| $\Gamma$ | Adsorbed amount (mass adsorbed per unit area of interface) |
| $D_m$ | *Mass* fractal dimension |
| $D_s$ | *Surface* fractal dimension |
| $D_f$ | Fractal dimension |
| $\xi$ | Fractal cut-off length |
| $\tau$ | Cluster polydispersity parameter (NB: smaller is broader!) |

Steve King
ISIS
October 2011

stephen.king@stfc.ac.uk

| No. | Model | Parameters | Equations | Remarks & References |
|---|---|---|---|---|

## SANSView Category: Shapes

| | | | | |
|---|---|---|---|---|
| 7 | I0 term for Second Moment of Adsorbed Layer (Complex)<br>(New_I0_Term)<br>(SIGMA2.FOR) | 1 Calibration factor<br>2 Density Poly [g/cm3]<br>3 Contrast Term [/cm2]<br>4 Core radius [Angs]<br>5 Vol fract/n of cores<br>6 Ads/d amount [mg/m2]<br>7 Second moment [Angs]<br>8 Background | $I_0(Q) \approx (\rho_l - \rho_m)^2 \times$<br>$\left[\frac{6\pi\phi_p}{Q^2}\frac{\Gamma^2}{\delta^2 R_p}\exp\left(-Q^2\sigma^2\right)\right] + B$ | "Using SANS to study adsorbed layers in colloidal dispersions" King, SM; Griffiths, PC; Cosgrove, T<br>Chapter 4 in "Applications of Neutrons in Soft Condensed Matter", Gabrys, BJ (editor) Gordon & Breach, (2000) |

This model, used in dozens of published papers, describes the scattering from a layer of surfactant or polymer adsorbed on spherical particles under the conditions that (i) the particles are contrast-matched to the dispersion medium, (ii) S(Q)~1 (ie, the particle volume fraction is dilute), (iii) the particle radius is >> layer thickness (ie, the interface is locally flat), and (iv) scattering from excess unadsorbed adsorbate in the bulk medium is absent or has been corrected for.

Unlike a core-shell model, this model does not assume any form for the density distribution of the adsorbed species normal to the interface (cf, a core-shell model which assumes the density distribution to be a homogeneous step-function). Parameter 7 is the *second moment about the mean* of the density distribution (ie, the distance of the centre-of-mass of the distribution from the interface). For comparison, if the thickness of a (core-shell like) step function distribution is $t$, the second moment $\sigma = (t^2/12)^{1/2}$.

A variant of this model allowing for polydispersity on the particle radius would be most welcome!

## SANSView Category: Shape-Independent

SANSView already incorporates a fractal aggregate model using Jose Teixeira's 1988 scattering function. However Teixeira and Chen developed this model further during the early 1990's. As the last reference shows, even Teixeira is still using it!

| | | | | |
|---|---|---|---|---|
| 24 | Chen Fractal Fit for Aggregates<br>(Chen)<br>(CHEN.FOR) | 1 Chen Fractal Scaling<br>2 Primary Radius [Ang]<br>3 Aggregation Number<br>4 Polyd of Cluster,Tau<br>5 Fractal Dimension Df<br>6 Background | $I(Q)=\frac{(\rho_{fractal}-\rho_{medium})^2\,.\,\Phi\,.\,V_{primary}\,.\,N_{agg}}{\Gamma(2-\tau)}\times$<br>$[F(3-\tau,Q\xi)\,(1+Q^2\xi^2)^{-D_f(3-\tau)/2}+$<br>$G(2-\tau,Q\xi)\left(\frac{Q\xi}{h}\right)^{-D_f}]+B$<br>Where<br>$V_{primary}=(4/3)\,.\,\pi\,.\,R_0^3$<br>$R_1^2=(3/5)\,.\,R_0^2$<br>$\xi=h\,.\,R_1\,.\,N_{agg}^{(1/D_f)}$<br>$h=\sqrt{\frac{D_f\;(D_f+1)}{6}}$<br>$F(a,x)=\Gamma(a)-\Gamma(a,u)$<br>$u=\left[\frac{h^2\,.\,(1+Q^2\xi^2)}{Q^2\xi^2}\right]^{D_f/2}$<br>$G(a,x)=\sin\left[\frac{(D_f-1)\,.\,\pi}{2}\right]\,.\,\frac{\Gamma\left(a,\left(\frac{x}{h}\right)^{D_f}\right)}{(D_f-1)}$ | Note that a *small* Polydispersity index corresponds to a *broad* size distribution.<br><br>Scaling is programmed as: $(\Delta\rho)^2.\Phi$<br><br>Chen, Rouch & Tartaglia Croat. Chem. Acta, 65(2), (1992), 353-366<br><br>Liu, Sheu, Chen & Storm Fuel, 74(9), (1995), 1352-1356<br><br>Fratini, Bonini, Oasmaa, Solantausta, Teixeira & Baglioni Langmuir, 22, (2006), 306-312 |

The following model is an alternative fractal aggregate model developed by Paul Schmidt, Dale Schaefer, and others.

| | | | | |
|---|---|---|---|---|
| 21 | Schmidt (Hurd-Schaefer-Martin) Mass & Surface Fractal<br>(Fractal_QtoN)<br>(QTON2.FOR) | 1 Prefactor Term<br>2 Mass Fractal Dimens.<br>3 Cluster Rg<br>4 Surface Fract. Dim.<br>5 Primary Rg<br>6 Background | $I(Q) = N.V^2.(\Delta\rho)^2.P(Q) + B$<br>Where:<br>$P(Q) = \{[1+(Q^2.a)]^{D_m/2} \times$<br>$[1+(Q^2.b)]^{(6-D_s-D_m)/2}\}^{-1}$<br>$a = R_g^2/(3.D_m/2)$<br>$b = r_g^2/[-3.(D_s-6+D_m)/2]$ | Note that $0 < D_s \leq 6$ and $0 < D_m \leq 6$.<br>Schmidt<br>J Appl Cryst<br>(1991), 24, 414-435<br>*See equation (19)*<br>Hurd; Schaefer; Martin,<br>Phys Rev A<br>(1987), 35, 2361-2364<br>*See equation (2)* |

The Teixeira model already in SANSView, and the Chen-Teixeira and Schmidt-Scaefer models above, are all fractal *aggregate* models. SANSView does not currently have any pure fractal scattering models. The following would remedy this situation.

| | | | | |
|---|---|---|---|---|
| 18 | Mildner-Hall Surface Fractal<br>(Fractal_Ds)<br>(DS.FOR) | 1 Prefactor Term<br>2 P(q) particle radius<br>3 Surface Fract. Dim.<br>4 Cut-off Length<br>5 Background | $I(Q) = N.V^2.(\Delta\rho)^2.P(Q,R).S(Q) + B$<br>Where:<br>$P(Q,R) = \left[\frac{3(\sin(QR) - QR\cos(QR))}{(QR)^3}\right]^2$<br>$S(Q) = [(\Gamma(5-D_s).\xi^{(5-D_s)}.[1+(Q^2\xi^2)]^{(D_s-5)/2} \times$<br>$\sin[(D_s-5).\arctan(Q\xi)]) / Q]$ | Note that $0 < D_s \le 6$.<br>Mildner; Hall,<br>J Phys D Appl Phys<br>(1986), 19, 1535-1545<br>*See equation (13)*<br>Triolo et al<br>J Appl Cryst<br>(2000), 33, 863-866<br>*See equation (3)* |
| 20 | Mildner-Hall (Schaefer-Keefer) Mass Fractal<br>(Fractal_Dm)<br>(DM.FOR) | 1 Prefactor Term<br>2 P(q) particle radius<br>3 Mass Fractal Dimens.<br>4 Cut-off Length<br>5 Background | $I(Q) = N.V^2.(\Delta\rho)^2.P(Q,R).S(Q) + B$<br>Where:<br>$P(Q,R) = \left[\frac{3(\sin(QR) - QR\cos(QR))}{(QR)^3}\right]^2$<br>$S(Q) = [(\Gamma(D_m-1).\xi^{(D_m-1)}.[1+(Q^2\xi^2)]^{(1-D_{ms})/2} \times$<br>$\sin[(D_m-1).\arctan(Q\xi)]) / Q]$ | Note that $0 < D_m \le 6$.<br>Mildner; Hall,<br>J Phys D Appl Phys<br>(1986), 19, 1535-1545<br>*See equation (9)*<br>Triolo et al<br>J Appl Cryst<br>(2000), 33, 863-866<br>*See equation (4)*<br>Schmidt<br>J Appl Cryst<br>(1991), 24, 414-435<br>*See equation (18)* |

As written above, the form factor contribution is assumed to be from spherical particles. This could, of course, be extended to other shapes.

The following model is useful for characterising gels/networks with different degrees of swelling.

| | | | | |
|---|---|---|---|---|
| 22 | Shibayama-Geissler Two-Length Scale Fit for Gels<br>(GelFit)<br>(GEISSLER.FOR) | 1 Lorenztian Scaling<br>2 Guinier Scaling<br>3 Short correl. Length<br>4 Radius of Gyration<br>5 Scaling Exponent<br>6 Background | $I(Q) = f.I(0)_1.\frac{1}{(1+[((D+1)/3).Q^2 a_1^2])^{D/2}} +$<br>$(1-f).I(0)_2.\exp(-Q^2 a_2^2) + B$<br>Where:<br>$D$ is the scaling exponent<br>$a_2^2 \approx \frac{R_g^2}{3}$<br>Note that this reduces to:<br>$I(Q) = f.I(0)_1.\frac{1}{(1+Q^2 a_1^2)} + (1-f).I(0)_2.\exp(-Q^2 a_2^2)$<br>when $D$=2; ie, when the Flory exponent is 0.5 (theta conditions) | Sibayama; Tanaka; Han<br>J Chem Phys<br>(1992), 97(9), 6829-6841<br><br>Mallam; Horkay; Hecht; Rennie; Geissler,<br>Macromol<br>(1991), 24, 543 |