**Subroutine: Chen**

Comparison data generated by program: Chen-prog.exe

This model describes the scattering from *polydisperse* fractal clusters of monodisperse non-interacting subunits (specifically, aggregates formed by a variable number of identical rigid spheres – primary ‘particles’ - that fill space according to the fractal power law RDf where 1 < Df < 3).

Note that *small* values of the polydispersity index τ correspond to a *broad* size distribution. A reaction-limited cluster aggregation (RLCA) process should lead to a τ value of 1.5.

The scattered intensity I(Q) is calculated as:



where:

 ; volume of a primary ‘particle’

 ; radius-of-gyration of a primary ‘particle’

 ; correlation length of the fractal cluster









Γ(a,u) is the incomplete Euler gamma function and Γ(a) is the normal gamma function.

REFERENCES

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YC Liu, EY Sheu, S-H Chen & DA Storm, Fuel, 74(9), (1995), 1352-1356

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TEST DATASET

This example dataset was produced using 300 data points, qmin=0.001 Å-1, qmax=0.3 Å-1 and the default values:

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter name | Symbol | Units | Default value |
| scale |  | cm-4 | 3.0X1019 |
| primary radius | R0 | Å | 3.5 |
| aggregation number | Nagg | None | 70.0 |
| cluster polydispersity | τ | None | 1.6 |
| fractal dimension | Df | None | 1.45 |
| background | B | cm-1 | 0.01 |

NB: The model could, of course, be parameterised by separating out the contrast term and volume fraction in the scale parameter.

The returned intensity is scaled to units of [cm-1].