Recovering porosity features from small angle X-ray (SAXS) measurements

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The Equation Free Summary:

For various reasons, there is a growing need to improve the technology for the extraction of energy from coal so that the energy recovered is maximized while the corresponding environmental impact is minimized. Because of the trade-off involved, such a goal can only be achieved through an explicit understanding and exploitation of the science of coal pyrolysis, liquefaction, gasification, char (solid material remaining after the removal of the light gasses and tars from coal) formation and char combustion.

As a direct consequence of the importance, over the centuries, of the extraction of energy from coal, the associated science and technology are already well understood and being exploited in various ways. However, the growing demands to minimize the impact on the environment of the associated energy extraction have spawned the need to improve on the current understanding of the science and technology.

In particular, this is leading to the need to address the following types of issues:

(a) The effect of pressure on coal pyrolysis and char formation.

(b) Char structure and reactivity.

(c) Modelling of the coal to char dynamics for different conversion strategies.

(d) Pilot scale gasification testing and the role of laboratory data.

In one way or another, in terms of the planning for future technological developments, all such issues involve the need to have an enhance understanding about the microstructure of coal and, because of its importance in the reactivity of coal and char, about the surface structure, the size distribution and surface area of the pores.
Clearly, for the recovery of information about such porosity features appropriate indirect measurements, such as small angle X-ray scattering (SAXS) measurements, must be utilzed. Even though the associated theory for SAXS measurements sits on a well published firm mathematical foundation, the demands for future planning are generating new questions which require investigation.
Consequently, for this MISG problem, CSIRO Energy Technology specifically requested that the recovery of porosity features from SAXS measurement be the focus of deliberations and requested that the following issues be given top priority by the study group.

(i) What is the nature of the inverse problem which relates porosity features to SAXS measurements?

(ii) To what extent should the fractral nature of the pores be taken into account?

(iii) Can the current algorithms for surface porosity estimation be improved?

(iv) How sensitive is the estimation of surface porosity to change of shape of the pores.

The success of the resulting deliberations led to the following outcomes:

1. The identification of where, in the equations that connected the porosity and SAXS measurements, the inverse nature of the connection is located.

2. The formulation of a functional strategy for estimating surface porosity from SAXS measurements.

3. A numerical procedure for the evaluation of the pore size distribution for different form factors.

4. The determination of the form factors for different pore geometries.

5. An uncertainty analysis of changing ellipsoidal shape.

6. A proof that the scattering by a fractal surface can be equivalenced with a polydisperse system of pores.