Outline of Problem for the 2012 UK Maths-in-Industry Study Group to be held in April 2012, at UEA, Norwich.

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A Model for the Reduction of Specific Surface Area of Powders with Age

High surface area powders are required in a number of technology areas. For example, the efficiency of catalysts is intimately linked to the surface area of the powder. In our context we are interested in explosives that are in the form of a powder. High surface area, small diameter powders tend to have a high Gibbs surface energy and tend to coarsen to reduce it. The main mechanisms by which powders may change their surface area are believed to be:

- evaporation-condensation, in which molecules detach from a particle surface, diffuse through the gas phase, and then condense on the surface of a different particle;
- surface diffusion, in which the molecule undergoes long-term diffusion on (solid) particle surfaces without detaching into the gas phase.

To date the mathematical modelling of the coarsening process, sometimes referred to as ‘Ostwald Ripening’, has usually made the assumptions that the explosives comprise a collection of detached spherical particles of differing radii and that mass transfer occurs via the Gibbs-Thompson effect. While the assumption of spherical shapes is a reasonable starting point, it is known that crystal growth is highly dependent on local surface curvature. It may be that postulation of a distribution of shapes might be a better way to improve the mathematical description of the process. In previous work correction factors are employed to account for particle shapes, surface roughness and the diffusion process. The first highly transient phase of the coarsening process in particular is still not very well understood.

The first main aim of the proposed study is to investigate the physical modelling of the atomic-level mass-transfer processes causing coarsening of solid powders, in particular addressing:

- how to relax the assumption of separate particles, instead allowing contact between them;
- and under these circumstances how to model evaporation-condensation and surface diffusion.

The next main aim is to model the evolution of the statistical distribution of particles, probably first assuming spherical particles and then relaxing that assumption. If possible it would be good to establish a flexible distribution model which would allow different models of the physical mechanisms to be tested.

AWE will supply a set of references on the physics and chemistry of the atomic mass-transfer processes and some data on particle distributions and explosive compositions. It is believed that there should be sufficient scope here to engage the academics over the week and to lead to some fruitful academic research. AWE experts will attend full-time to assist with obtaining information and to decide on priorities, etc.