Comppro: Solids

Here are some notes I made (hence the mistakes are mine so far!) from yesterday's meeting – please indicate additions to/ arguments against/ amendments, before we circulate a 'finished' document from the Modelling of Solids Phase Processing Workshop.

General points:
It was suggested that there was less coherency in the modelling of solid polymer processing than in the case of melt processing – because of the morphology/ structure issues, in addition to purely molecular issues?

- there is more to cover in the case of solids.
- there is general agreement over the philosophy/ global matters, but more ad hoc approaches are followed in the details. Perhaps we cannot expect generality – different materials will require different features in modelling of their deformation behaviour?
- there is a set of tools for modelling solid phase deformation, however, the details of the tools will differ for different materials, as indicated in points below
- continuum approaches may be ok for engineering solutions, but there will be increasing need for more specific, structurally-related approaches
- We are currently not in a position to predict *a priori* the deformation behaviour of polymers
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What are the main areas of progress in modelling of solid phase processing of polymers?

- constitutive equations for use in numerical methods, which now incorporate strain and strain rate dependence. All groups (?) have network and rate dependence
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What are the current gaps in our ability to model solid phase processing of polymers?
Constitutive equations - Structural issues:

- incorporation of detailed structural modelling will be increasingly required;
- a continuum approach is probably ok for amorphous polymers – ok in equilibrium, at T>Tg (when they behave more like fluids!)
- phase transitions & their rheological consequences need to be handled
- we currently have to extrapolate constitutive equations to processing regime conditions.

Experimental issues:

- we need techniques which provide data relevant to processing operations;
- more detailed in-process measurements would be beneficial (especially if these could detect structure issues)

Numerical techniques:

- The community represented at the meeting made large use of ABAQUS, particularly because of its UMAT capabilities (but which were recognised as requiring considerable programming input)
- Some groups have their own code: Loughboro' indicated their approach, aiming at a new numerical scheme which could also handle phase change; it was queried if Physica (Mark Cross et al, Greenwich) could be considered as similar.
- If more complex constitutive equations are introduced, might this lead to significant difficulties in the numerical solvers?
- The potential for Lagrangian solvers might be explored (cf. the melts work of Harlen [though this involves a Eulerian-Lagrangian solver])