# Chemical Engineering Seminars – HT 2007

***Week 5: Tuesday 13 February, 4:15-5.15 pm***
***Lecture Room 2, Thom Building, Engineering Science***

## Efficient modelling of phase equilibria of polydisperse polymer systems


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**Abstract**


Accurate prediction of the phase equilibria of polymers and polymer mixtures requires thermodynamic models which are able to deal with large size differences between molecules and strong deviations from ideal behaviour over wide ranges of operating conditions. However, most polymers of industrial interest are polydisperse, with their molecular weight being distributed over a wide range of values. The corresponding thermodynamic behaviour and properties depend continuously on their molecular weight distribution. A standard approach is to assume a mathematical form for the distribution and then to discretise it into a certain number of pseudo-components. This often leads to problems relating to the efficient handling of large number of pseudo-components and the potentially small concentrations of some pseudo-components in one or more phases, especially in view of the fact that advanced equations of state such as SAFT are already highly nonlinear.

In this talk, a new methodology for phase equilibrium calculations of polydisperse polymers is presented. Given a polymer characterised by a set of measurable quantities, an automatic optimisation-based algorithm is used to determine an accurate and computationally efficient discrete representation of the molecular weight distribution. The phase equilibrium problem for the polydisperse system is then solved via a homotopy/continuation algorithm making use of a physical continuation parameter corresponding to the polymer polydispersity. Starting from the corresponding monodisperse system, the homotopy continuously deforms the system to the desired polydisperse representation, while satisfying certain constraints throughout its path. The algorithm is applied to liquid-liquid equilibria problems and is shown to be accurate and reliable irrespective of the number of pseudo-components introduced by the discretisation..


**Bio-sketch**

**Dr Kakalis** was awarded his Diploma in Metallurgical Engineering from the National Technical University of Athens in 2000. He followed this with an MSc and PhD in Process Systems Engineering, Centre for Process Systems Engineering, Imperial College London. He is now a post-doctoral research fellow with the Fluidics & Biocomplexity Group at the Department of Engineering Science, University of Oxford.