The CDS implementation of the DETHERM Thermophysical Database in the Imperial Chemical Engineering Department – Amparo Galindo (a.galindo@ic.ac.uk)

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I work as a Lecturer in the Department of Chemical Engineering and Chemical Technology in Imperial College London, and I am also an Advanced Research Fellow of the EPRSC. The research interests of my group focus on the development of statistical mechanical approaches for complex systems, and their application to processes relevant to industry. Our interest in this field is to develop fundamental approaches to contribute to the understanding of experimental systems, with a special focus on chemical processes. The goal is to be able to truly predict complex phase behaviour. The types of problems we are interested in at the moment include charged systems, near-critical and supercritical separations, mixtures of polymers and liquid crystals, and solid phases of chain molecules. The impact and exposure of this work is maximised through collaborative efforts in which the aim is to promote the transfer of the theoretical developments into tools for the design and synthesis of chemical processes and products. In carrying out this work we rely ultimately on experimental information of thermodynamic properties of the systems of interest: sometimes to correlate the parameters in our models, and sometimes to assess the accuracy of our theoretical predictions.

Although we collaborate within and outside the UK with groups involved in experimental work, in most cases the data we use is from previous published work. The search for accurate and relevant data can become an intensive task, and in this sense the Chemical Database has become an invaluable tool in our group. It saves incredible amounts of time to have on-line access to such a compilation of information. Two especially useful characteristics of the database are that it provides full references to the sources of the data for verification and assessment of experimental techniques, and that the data can be tabulated or formatted into graphic form and transported electronically directly into Windows or Linux packages.

Patel BH, Paricaud P, Galindo A, Maitland GC (2003) “Prediction of the salting-out effect of strong electrolytes on water plus alkane solutions”, *Ind. Eng. Chem. Res,* **42, .**3809-3823