Solvent selection for sustainable chemical development

Paul Murray Catalysis Consulting

Dr Paul Murray

email: paul.murray@catalysisconsulting.co.uk

Web: www.catalysisconsulting.co.uk

Solvents play a very significant role in many chemical reactions. Many common solvents have significant environmental, health or safety concerns related to them. A number of solvent selection guides have been published in recent years including the ACS Green Chemistry Institute Pharmaceutical Roundtable.

The selection of the correct solvent can afford cleaner reactions with higher selectivity's and higher yields. Solvent choice has even been found to completely change the selectivity of some reactions.

Solvent selection can be simplified by using Principal Component Analysis (PCA). Combining PCA with Design of Experiments (DoE) allows the investigation of solvent effects alongside the development of a reaction and the investigation of significant factors. PCA then allows the identification of the solvent properties required to achieve the best reaction. This in turn assists the selection of the best solvent for a process based on environmental, health and safety concerns alongside the bulk availability and cost. Solvent selection assisted by PCA enables the efficient development of sustainable chemical processes through informed decision making.

In this presentation, specific examples of where solvent choice has benefited process efficiency and performance will be discussed to highlight the impact of moving to more sustainable chemicals, and case examples of the successful use of PCA which have industrial application.