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INTEGRATING PROCESS AND MOLECULAR DESIGN: A JOURNEY ACROSS SCALES

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Abstract: The performance of chemical processes depends not only on flowsheet structure, equipment design and operating conditions, but also on the choice of processing materials such as catalysts and solvents. Using a different solvent, for instance, can change the rate of a reaction by several orders of magnitude. Despite this, processing materials are often selected very early process development, leading to sub-optimal process performance.
In this seminar, we explore how better designs can be developed by integrating molecular and process design decisions. Given the number of potential solutions to this extended design problem, and the complexity of the task, computer-aided design techniques and multiscale models have an important role to play in identifying promising options, thereby providing focus for experimental studies. We highlight the key challenges that must be overcome to enable such multiscale design and demonstrate what can be achieved on different processes.

Bio: Claire Adjiman is Professor of Chemical Engineering at Imperial College London. She holds an MEng from Imperial College and a PhD from Princeton University. Her interests centre on integrated process and molecular design, including new techniques for property prediction and optimisation. She is a Fellow of the Royal Academy of Engineering, the Institution of Chemical Engineers and the Royal Society of Chemistry. She sits on the editorial boards ofMolecular Systems Design & Engineering, Computers & Chemical Engineering and Fluid Phase Equilibria and is associate editor of the Journal