Imperial College London

Centre for Process Systems Engineering
2017 Seminar Series

UCL

Mathematical Optimization for Process Operations and Materials Design

Prof. Chrysanthos E. Gounaris

(Carnegie Mellon University)

Abstract:

In this talk, we introduce and motivate a number of practically interesting problems that arise in the areas of process scheduling and distribution logistics. We then derive various mathematical models and, since such operations are combinatorially complex and usually intractable to address with commercial optimization software, we develop custom-built optimization algorithms in order to obtain optimal decisions.

A common underlying theme of the above problems is the multi-stage nature of the decision-making they involve, whereby an operator can defer certain decisions until later time points. In these settings, it is of interest to derive solutions that maintain their feasibility across long time horizons and across a wide range of possible variability for the system parameters. It is also of interest to ensure that any solution one adopts remains competitive under many scenarios and is not subject to an unnecessarily excessive amount of risk premium. In this context, we apply and extend various principles and methodologies of Robust Optimization (RO) to manage such risk due to parameter uncertainty, and we show how novel RO frameworks can be used to improve upon solutions obtained via traditional means, including cases where traditional RO is not applicable.

Finally, we discuss recent efforts towards the design of heterogeneous catalyst systems where, due to the combinatorial nature of how atoms can arrange themselves on crystalline lattices, the best catalytic structures are often unintuitive and likely impossible to identify without a rigorous decision-making approach. To that end, we formalize a mathematical optimization approach for materials design and show how correlations linking catalytic activity to appropriate site descriptors can be used to determine the most promising designs of transition metal crystalline surfaces. Our results show that careful nanostructuring of these surfaces can dramatically enhance performance as compared to the various crystallographic planes that are more commonly used.

Bio:

Professor Chrysanthos Gounaris received a Dipl. in Chemical Engineering (2002) and an M.Sc. in Automation Systems (2003) from the National Technical University of Athens. He then attended Princeton University, where he earned an M.A. (2005) and a Ph.D. in Chemical Engineering (2008). His doctoral thesis, pursued under the supervision of Professor Chris A. Floudas, explored the use of nonlinear modeling and global optimization techniques to study porous materials. After graduation, Professor Gounaris joined McKinsey & Co. as an Associate, where he provided consultation to petrochemical, pharmaceutical and consumer packaged-goods companies on a variety of projects of operational and strategic nature (2008 -2010). He returned to academia to pursue post-doctoral research at Princeton University (2010-2013), after which he joined the Department of Chemical Engineering at Carnegie Mellon University as an Assistant Professor (2013-).

21 November, 11am
CPSE Seminar room, RODH C615

CPSE Seminar room, RODH C615, Roderic Hill Bldg, Chemical Engineering department, Imperial College London, SW7 2AZ
This event is free and open to the public. No registration is required.
Refreshments before the seminar in CPSE Common room (top floor Roderic Hill Bldg).

Organisers & Contacts: Dr. Gonzalo Guillen (g.guillen05@imperial.ac.uk), Dr. Alex Kiparissides (alex.kiparissides@ucl.ac.uk), Ms. Cristina Romano (c.romano@imperial.ac.uk)