ΕΘΝΙΚΟ ΜΕΤΣΟΒΙΟ ΠΟΛΥΤΕΧΝΕΙΟ
ΣΧΟΛΗ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ

ΕΠΙΤΡΟΠΗ ΣΕΜΙΝΑΡΙΩΝ, Καθηγητής Α. Κοκόσης

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ΣΕΜΙΝΑΡΙΟ ΧΗΜΙΚΗΣ ΜΗΧΑΝΙΚΗΣ

Πέμπτη 22 Απριλίου, 13:00

Αίθουσα Σεμιναρίων «Ν. Κουμούτσου»

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A Process Systems Engineering Approach for Managing the Complexity in Chemical Product-Process Design

Chemical product-process design consists of finding the identity of the candidate chemical product, designing the process that can sustainably manufacture it and verifying the performance of the product during application. The chemical product tree is potentially very large; starting from a set of basic raw materials (such as petroleum, biomass, coal, natural gas, rock, etc., that are usually extracted), to a bigger set of basic chemical products (such as, ethylene, benzene sulfuric acid, ammonia, etc., that are produced in large quantities), to an even bigger set of intermediates (such as, methanol, urea, succinic acid, ethylene glycol, etc., that are produced from the basic chemicals), to a very large number of refined chemicals and consumer products (where the chemical selected as the active ingredient is usually used in small quantity). At the top, the chemical products are usually from the life sciences, pharmaceutical, food and related industries and their development is principally based on experiment-based trial and error approaches. At the lower-middle end, the chemical products usually from the oil, petrochemical and chemical industries and use of model based tools in their development is quite common. however, unlike the oil and petrochemical industries in the life sciences, pharmaceutical, food and related industries, problems associated with product-process design and development involve several distinct features: *Multi-scale* (important data related to the chemicals come from different sources, at different scales of size and time); *Multidiscipline* (knowledge/data regarding the conversion of the biomaterial and/or intermediate chemicals from different disciplines); *Computer-aided techniques* (lack of models to predict the behaviour of the chemicals at different scales, of enzymes during organic synthesis, of reaction kinetics, etc., means that appropriate model-based techniques have not been developed).

Based on the above discussion it can be noted that methods and tools for current and future product-process design and development need to manage complex situations requiring handling of data and knowledge from different sources and at different scales of time and size. Use of a systems approach that can efficiently *manage the complexity* therefore becomes desirable. The principal idea here is to decompose a complex problem into a set of sub-problems that are easier to solve and to identify those that can be solved through model-based solution approaches. This solution approach helps to reduce the search space through each subsequent sub-problem solution and is able to find truly innovative solutions to the design problem. Only at the last (validation) step, experiments or rigorous simulation is performed. The advantage of this combined hybrid (systems approach) is that during the early stages, where enough data and models are available (or could be easily generated), the search space is rapidly reduced while the resources for experiments are used for final selection of the product.

The lecture will present the main concepts, the use of these concepts in a model based framework to manage the complexity together with illustrative examples highlighting the application of the model-based framework.