> Seminario de Matemática Aplicada

USC UNIVERSIDADE DE SANTIAGO DE COMPOSTELA — DEPARTAMENTO DE MATEMÁTICA APLICADA

imat

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Incremental model identification of reaction systems

The identification of reaction kinetics represents the main challenge in building models for reaction systems. The identification task can be performed via either simultaneous model identification (SMI) or incremental model identification (IMI), the latter using either the differential (rate-based) or the integral (extent-based) method of parameter estimation.

In SMI, a rate law must be postulated for each reaction, and the modeled concentrations are obtained by integration of the balance equations. The procedure must be repeated for all combinations of rate candidates. This approach is computationally costly when there are several candidates for each reaction, and convergence problems may arise due to the large number of parameters.

In IMI, the identification task is decomposed into several sub-problems, one for each reaction. Since IMI deals with one reaction at a time, only the rate candidates for that reaction need to be compared. In addition, convergence is facilitated by the fact that only the parameters of a single reaction rate are estimated in each sub-problem. In extent-based IMI, the simulated rates are integrated to yield extents, and the parameters are estimated by fitting the simulated extents to the experimental extents obtained by transformation of measured concentrations.

In this talk, different cases of reaction systems will be presented, the concept of extents will be discussed for each case, and we will show how extents can be obtained from concentrations via linear transformation. Then, the decoupling provided by the concept of extents will be applied to incremental model identification of these reaction systems, which allows correct model discrimination and accurate parameter estimation.

Data	**Mércores, 29 de marzo de 2017**
Lugar	**Salón de Graos - Facultade de Matemáticas**
Hora	**12:30**
Idioma	**Inglés**

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