

Workshop on
Structural Identifiability Analysis in Chemical Engineering and Tribology
EPFL, Room MXC315, June 20-21, 2013

Organizers:

Prof. A. Igual Muñoz, Polytechnic University Valencia (UPV), Host professor EPFL
Dr MER S. Mischler, Tribology and Interface Chemistry, IMX- EPFL

Invited speaker

Javier Navarro Laboulais, Polytechnic University Valencia (UPV)

ABSTRACT

Mathematical modelling in engineering is needed to understand and predict the behaviour of systems. These models should be experimentally "tuned" by observing the response of the output variables against the modification of some operational (input) variables. Specific mathematical tools, such as Structural Identifiability, allow the *structural analysis* of the numerical model as a tool to rationalize experiments.

The Structural Identifiability of mathematical models seeks for: i) identifying the maximum number of parameters which could be determined for a given set of input-output data; ii) determining which model will give the maximum information of the system when several models explain the same phenomenon for the same set of input-output data, iii) enabling an optimal design of experiments by selecting a number of state variables.

Tribology is the science of friction, lubrication and wear. Tribological contacts are complex systems, i.e. of dissipative nature and controlled by a large number of variables. Research in tribology has been mainly addressed by using a heuristic approach that shows now clear shortcomings due to the variability and instability of the involved phenomena. Indeed, despite two centuries of research efforts, no general theories for friction or wear exist.

The aim of this workshop is to explore possibilities to apply Structural Identifiability to tribological systems. The workshop is divided in three parts. In the first day, some mathematical techniques for structural and practical identifiability analysis of models will be introduced. Their application to heterogeneous chemical processes for wastewater ozonation biological systems, and general first order chemical reactions will be discussed. In the second part, the basic concepts of tribology and some related cases studies will be presented. The potentiality of new mathematical tools in tribology will be appraised during a final round table discussion.

Participation is free. Guests are welcome.

PROGRAM

Part 1: 20 June 2013, Room MXC315

Structural Identifiability Analysis in Chemical Engineering (Chair: A. Roda Buch)

10:00 Welcome Prof. A. Igual Munoz, S. Mischler

10:15 Theoretical framework (J. Navarro, UPV)

11:15 Break

11:45 Case studies: Heterogeneous Chemical Reactors (J. Navarro, UPV)

12:45 End of Part 1

Part 2: 21 June 2013, Room MXC315

Tribology case studies (Chair: A. Igual Muñoz)

09:15 Introduction to tribology (S. Mischler, EPFL)

09:45 Case study 1: Tribocorrosion of CoCrMo alloys (S. Guadalupe, EPFL)

10:15 Break

10:45 Case study 2: Abrasion in simulated wheel-rail contacts (A. Roda Buch, UPV/EPFL)

11:45 End of Part 2

Part 3: 21 June 2013, Room MXC315

Structural Identifiability Analysis in Tribology (Chair A. Igual Muñoz, Dr S. Mischler)

12:00 Round table discussion on possible applications of Structural Identifiability Analysis in Tribology

12:45 End of part 3

INVITED SPEAKER

Javier NAVARRO-LABOULAIS obtained B.Sc. (1989) in Chemistry, M.Sc. (1990) in Physical Chemistry and Ph.D (1998) in Chemistry, all from the University of Valencia. Currently, he holds a position of Lecturer in Chemical Engineering in the Chemical and Nuclear Engineering Department at the Polytechnic University of Valencia and he is a member of the Institute for Industrial, Radiophysical and Environmental Safety at the same University.

He has research interests in the mathematical modelling of chemical kinetic and mass transport processes ranging from electrochemical systems, to heterogeneous gas-liquid mass transfer processes, ozonation and related advanced oxidation techniques and biokinetic parameters determination in wastewaters. His interests also include experimental techniques associated to these technologies such as data acquisition systems, automation, control and data analysis.

Related publications

Navarro-Laboulais, J., Cardona, S. C., Torregrosa, J. I., Abad, A., López, F. (2006). *Structural identifiability analysis of the dynamic gas-liquid film model*, AIChE J., 52, 2851-2863.

Navarro-Laboulais, J., Cardona, S. C., Torregrosa, J. I., Abad, A., López, F. (2008). *Practical identifiability analysis in dynamic gas-liquid reactors: Optimal experimental design for mass-transfer parameters determination*, Comput. Chem. Eng., 32, 2382-2394.

Navarro-Laboulais, J., López, F., Torregrosa, J.I., Cardona, S.C., Abad, A. (2007) *Transient Response, Model Structure and Systematic Errors in Hybrid Respirometers. Structural Identifiability Analysis Based on OUR and DO Measurements*; J. Math. Chem. 42, 969-90

Cantó, B., Coll, C., Sánchez, E., Cardona, S.C., Navarro-Laboulais (2013); *On identifiability for chemical systems from measurable variables*; J. Math. Chem. DOI 10.1007/s10910-013-0149-4