Course Title: Introduction to mathematical modeling

Modality: CFT- Transversal Training Course

Orientation:

- ☐ Ocean Observation and Global Change
- ☐ Sustainable use of Marine Resources
- ☐ Integral Management of the Sea
- ☐ Technological progress. Engineering and Business Management

Dates: 11/05/2020; 12/05/2020

Timetable: 9:30h

Duration: Around 7 hours

Location: Instituto de Investigaciones Marinas / Aula DO*Mar

Language: English/Spanish/Portuguese

Academic coordinators:

Name	Institution	e-mail
Eva Balsa-Canto	IIM-CSIC	ebalsa@iim.csic.es

Lecturers:

Name	Institution	e-mail
Antonio Álvarez Alonso	IIM-CSIC	antonio@iim.csic.es
Lino Santos	FCTUC	lino@eq.uc.pt

General description:

Introduction to first principles based mathematical modeling (mass, energy and momemtum conservation laws). Numerical methods to solve ordinary differential equations (ODEs) and partial differential equations (PDEs). Numerical examples in Matlab.

Contents:

- Description of transport phenomena and biotransformation
- Introduction to the dynamic simulation. Discretization methods. Predictor-corrector methods.

- Introduction to the simulation of distributed systems. Numerical methods to solve partial differential equation systems. Finite differences method as an example.
- Modeling and simulation of homogeneous and distributed (bio-)processes. Illustrative examples.

Teaching methodologies:

The teaching will be made using PowerPoint presentations, chalk board and presentations of computer simulation in Matlab.

Evaluation system:

The grading is based on a short report on modeling and simulation of given system written by the student. The dynamic system case study is of the choice of the student. The report comprises the description of the dynamic, the formulation of the mathematical model, and the description of the numerical strategy (numerical tools, solvers, etc.) to solve the model.

Briev CV of the lecturers:

Dr Antonio A. Alonso is a Research Professor at the Spanish Council for Scientific Research, and a member of the Process Engineering Group within the Food Science and Technology Department at the IIM-CSIC (Instituto de Investigaciones Marinas) in Vigo, Spain. Before joining the CSIC in 2001, Dr Alonso hold a position as Associate Professor of Chemical Engineering at the University of Vigo. He has a B.Sc Chemistry University of Santiago de Compostela (1984-1989), Industrial Chemistry and a PhD in Chemical Engineering, by the same University (1993).

His research activity lies within the area of Process and Bioprocess Engineering, with contributions in the field of mathematical modeling, computer-aided simulation, optimization and robust and predictive control. Particular research interests include modeling and model reduction of distributed process systems described by mass, energy and momentum, analysis of chemical and biochemical reaction networks, and real time robust decision-making tools for processes and bioprocesses.

Some selected publications

Pájaro, M., Otero-Muras, I., Vazquez, C., Alonso, A.A.(2019) Transient hysteresis and inherent stochasticity in gene regulatory networks. Nature Communications 10 (1): 4581

García, M.R., Vazquez, J.A., Teixeira, I.G., Alonso, A.A. (2018) Stochastic individual-based modelling of bacterial growth and division using flow Cytometry. Frontiers in Microbiology 8: 2626

Pájaro, M., Otero-Muras, I., Vazquez, C, Alonso A.A. (2018) SELANSI: a toolbox for simulation of

stochastic gene regulatory networks. Bioinformatics 34(5): 893-895

Vilas, C., Alonso, A.A., Herrera, J.R., Garcia-Blanco, A., García, M.R.(2017) A model for the biochemical degradation of inosine monophosphate in hake (Merluccius merluccius). Journal of Food Engineering 200: 95-101

Alonso, A.A. Szederkenyi, G. (2016) Uniqueness of feasible equilibria for mass action law (MAL) kinetic systems. Journal Process Control 48: 41-71

Pajaro, M., Alonso, A.A. Vazquez, C. (2015) Shaping protein distributions in stochastic self-regulated gene expression networks. Physical Review E 92: 032712

Alonso, AA, Molina, I., Theodoropoulos, C. (2014) Modeling bacterial population growth from stochastic single-cell dynamics. Applied and environmental microbiology 80 (17): 5241-5253

Alonso A.A., Arias-Mendez, A., Balsa-Canto, E., Garcia, M.R., Molina, J.I., Vilas, C., Villafin, M. (2013) Real time optimization for quality control of batch thermal sterilization of prepackaged foods. Food Control 32(2): 392-403

Garcia, M.R., Vilas, C., Santos, L.O., Alonso, A.A. (2012) A robust multimodel predictive controller for distributed parameter systems. Journal of Process Control. 22: 60-71

Otero-Muras, I., Banga, J.R., Alonso, A.A (2012) Characterizing multistationarity regimes in biochemical reaction networks. PLoS ONE 7(7): e39194

Dr. Lino Santos is Auxiliary Professor at the Department of Chemical Engineering of the Faculty of Sciences and Technology of the University of Coimbra, Portugal. He has a licenciate's degree (1990) and a Ph.D. (2001) in Chemical Engineering from the University of Coimbra. Dr. Santos's teaching Chemical Engineering undergraduate courses include the course of Supervision of Processes, that covers topics in process dynamics, process control, mathematical modeling, and computer simulation. His research activity lies in the area of process modeling and control. Current research activities are in the area of nonlinear model predictive control, and process modeling and optimization.

Some selected publications

Amador A., Fernandes F.P., Santos L.O., Romanenko A., Rocha A.M.A.C. (2018) Parameter Estimation of the Kinetic α-Pinene Isomerization Model Using the MCSFilter Algorithm. In: Gervasi O. et al. (eds) Computational Sience and Its Applications – ICCSA 2018. ICCSA 2018. Lecture Notes in Computer Science, vol 10961. Springer, Cham

Brásio, A.S.R., Romanenko, A., Fernandes, N.C.P., Santos, L.O. (2016). First principle modeling and predictive control of a continuous biodiesel plantJournal of Process Control, Journal of Process

Control, 47, 11-21

Dewasme, L., Fernandes, S., Amribt, Z. Santos, L.O., Bogaerts, P., Vande Wouwer, A. (2015). State estimation and predictive control of fed-batch cultures of hybridoma cellsJournal of Process Control, Journal of Process Control, 30, 50-57

L. O. Santos, L. Dewasme, D. Coutinho, A. Vande Wouwer (2012). Nonlinear model predictive control of fed-batch cultures of micro-organisms exhibiting overflow metabolism: assessment and robustness. Computers & Chemical Engineering, 39, 143-151

M. R. García, C. Vilas, L. O. Santos, A. A. Alonso (2012). A robust multimodel predictive controller for distributed parameter systems. Journal of Process Control, 22, 60-71

L. O. Santos, L. Dewasme, A.-L. Hantson, A. Vande Wouwer (2010). Nonlinear model predictive control of fed-batch cultures of micro-organisms exhibiting overflow metabolism. 2010 IEEE Multi-Conference on Systems and Control (MSC), Yokohama, Japan, pp. 1608-1613

L. O. Santos, L. T. Biegler, J. A. A. M. Castro (2008). A tool to analyze robust stability for constrained nonlinear MPC. Journal of Process Control, 18, 383-390

A. Romanenko, L. O. Santos, P. A. F. N. A. Afonso (2004). Unscented Kalman Filtering of a Simulated pH System. Industrial & Engineering Chemistry Research, 43, 7531-7538

L. O. Santos, P. A.F.N. A. Afonso, J. A.A.M. Castro, N. M. C. Oliveira, L. T. Biegler (2001). On-line implementation of nonlinear MPC: an experimental case study. Control Engineering Practice, 9, 847-857

Relevant references:

Hangos, K., Cameron, I. (2001). Process Modelling and Model Analysis, 4th vol. of Process Systems Engineering, Academic Press, San Diego, CA

Chapra, S. (2005). Applied Numerical Methods with MATLAB for Engineers and Scientists, McGraw-Hill, Boston, MA

Mangel, M (2007) The Theoretical Biologist's Toolbox: Quantitative Methods for Ecology and Evolutionary Biology, Cambridge

Vande Wouwer, A., Saucez, P., Vilas, C. (2014). Simulation of ODE/PDE Models with MATLAB, OCTAVE and SCILAB, Springer, Cham

The MathWorks Inc. (n.d.). MATLAB Documentation. Retrieved from https://www.mathworks.com/help/matlab/index.html