

## CFT 2: INTRODUCCIÓN AL MODELADO MATEMÁTICO

**Fecha:** 01-02 Febrero 2016

**Horario:** día 1: 9:30-13:00  
día 2: 9:30-14:00

**Tipo de curso:** Curso teórico

**Lugar:** Aula de videoconferencia Edificio CITE XVI, Universidade de Vigo

**Coordinadora:** Eva Balsa-Canto, IIM-CSIC ([ebalsa@iim.csic.es](mailto:ebalsa@iim.csic.es))

**Profesores:** Antonio Álvarez Alonso (IIM-CSIC)  
Lino Santos (Universidade Coimbra)

### DESCRIPCIÓN

Introducción al modelado matemático basado en primeros principios (conservación de la masa, momento y energía). Métodos numéricos para la resolución de ecuaciones diferenciales y en derivadas parciales. Casos prácticos en MATLAB.

### Contenidos

- Descripción de fenómenos de transporte y biotransformación
- Introducción a la simulación dinámica. Métodos de discretización en el tiempo. Métodos predictores-correctores.
- Introducción a la simulación de sistemas distribuidos. Métodos numéricos de resolución de ecuaciones en derivadas parciales. Diferencias finitas como ejemplo.
- Modelado y simulación de (bio-)procesos homogéneos y distribuidos. Casos prácticos.

### Programa docente (sesiones temáticas y otras actividades)

El curso se organizará en dos sesiones de 3 y 4 horas respectivamente.

- En la primera sesión el Prof. Santos abordará la descripción de fenómenos de transporte y biotransformación y realizará una introducción a la simulación dinámica, a los métodos predictores-correctores. Sesión de 3 horas.
- En la segunda sesión el Prof. Alonso presentará una introducción a la simulación de sistemas distribuidos y a los métodos numéricos para su resolución. Sesión de 2 horas. A continuación ambos profesores presentarán ejemplos prácticos de modelos dinámicos de sistemas homogéneos y distribuidos. Sesión de 2 horas.

## Metodología docente

Presentación en Powerpoint y pizarra. Los ejemplos se ilustrarán utilizando MATLAB.

## Sistema de Evaluación

Los alumnos desarrollarán un trabajo breve. Como propuesta inicial se plantea la posibilidad de que cada alumno seleccione un modelo dinámico de su interés y plantee la metodología más adecuada para su resolución.

## Profesores del curso

### Dr. Lino Santos

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.

- Brásio, A.S.R., Romanenko, A., Leal, J., Santos, L.O., Fernandes, N.C.P. (2013). Nonlinear model predictive control of biodiesel production via transesterification of used vegetable oils. *Journal of Process Control*, 23 (10), pp. 1471-1479
- 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 (2007). A nonlinear model predictive control framework as free software: outlook and progress report. *Assessment and Future Directions of Nonlinear Model Predictive Control*, R. Findeisen, F. Allgöwer, and L. Biegler (Eds.), LNCIS 358, Springer, Berlin, 229-238
- 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

Dr. Antonio A. Alonso

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. During the last years he participated and coordinated a number of national and EU funded research projects in the areas of food technology and process engineering, covering subjects related with plant wide process control and design. Most projects he participates in are related to the development and implementation of efficient process system engineering tools to improve the operation of bioprocesses. As a result of his research activity he has published over 200 publications including articles, book chapters and congress proceedings.

Some selected publications

- Alonso, A.A., Ydstie, B.E.. (2001) Stabilization of Distributed Process Systems Using Irreversible Thermodynamics. *Automatica*. 37(11): 1739-1755
- Alonso, A. A., Vilas, C., Banga, J.R. (2004) Dissipative systems: from physics to robust nonlinear control. *Int. J. Robust & Nonlinear Contr.* 14. 157-179
- Alonso AA, Frouzakis CE, Kevrekidis IG (2004) Optimal sensor placement for state reconstruction of distributed process systems. *AIChE Journal*. 50 (7) : 1438-1452
- Vilas C, Garcia MR, Banga JR, Alonso AA (2006) Stabilization of inhomogeneous patterns in a diffusion-reaction system under structural and parametric uncertainties. *Journal of Theoretical Biology*. 241 (2) : 295-306
- Antelo, L. T., Otero-Muras, I., Banga, J.R., Alonso, A. A (2007) A systematic approach to plant-wide control based on thermodynamics. *Computers & Chemical Engineering* . 31(5-6): 677-691
- Otero-Muras, I., G. Szederkényi, K.M. Hangos and A. A. Alonso (2008) Local dissipative Hamiltonian description of reversible reaction networks. *Systems and Control Letters*. 57: 554-560
- Garcia, M.R., Vilas, C., Banga, J.R., Alonso, A. A (2008) Exponential Observers for Distributed Tubular (Bio)Reactors. *AIChE J.* 54(11): 2943-2953
- Otero-Muras, I., Banga, J.R., Alonso, A.A. (2009) Exploring Multiplicity Conditions in Enzymatic Reaction Networks. *Biotechnology Progress*. 25 (3) : 605-904
- Alonso, A.A., Antelo, L.T., Otero-Muras, I., Perez-Galvez, R.(2010) Contributing to Fisheries sustainability by making the best possible use of their resources: the BEFAIR initiative. *Trends in Food Science and Technology*. 21: 569-578
- 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
- AA Alonso, I Molina, C Theodoropoulos (2014) Modeling bacterial population growth from stochastic single-cell dynamics. *Applied and environmental microbiology* 80 (17), 5241-5253
- M R García, CV Fernández, JJ R Herrera, M Bernárdez, E Balsa-Canto, AA Alonso (2015). Quality and Shelf-life Prediction for Retail Fresh Hake (*Merluccius merluccius*). *International Journal Food Microbiology* vol.:208 pág.:65 -74.