

RESEARCH PROFILE AND PUBLICATIONS (2005-2010)

Mathematical modelling, simulation, optimization and control of bioprocesses

The main overall objective of this research line is to improve the efficiency of bioprocesses via **systems engineering** methods. These methods are based on a model-driven systemic approach, i.e. they make extensive use of **mathematical models and simulation, optimization and control methods and tools (software)**.

The ultimate goal is to improve the efficiency of these processes and the quality and safety of their products, reducing energy and water consumption and environmental impact.

There are two main blocks of objectives:

1. **methods**: to develop robust and efficient methods and tools (software) for the multi-scale mathematical modeling, **simulation, optimization, monitoring and control of bioprocesses**
2. **applications**: to apply these methods and tools to real processes and systems of clear interest, such as industrial processes of high economic importance (food and biotechnological sectors), and relevant biosystems associated with them (**systems biology of microorganisms**)

2010

Papers in Journals

J. ROSS, A. FERNÁNDEZ VILLAYERDE, S. VÁZQUEZ, J.R. BANGA, F. MORÁN. Julio 2010. A generalized Fisher equation and its utility in chemical kinetics. *Proceedings of the National Academy of Sciences of the USA*. 107: 12777-12781

BALSA-CANTO, E., A.A. ALONSO, BANGA, J.R. 2010. An iterative identification procedure for dynamic modelling of biochemical networks. *BMC Systems Biology*.4:11.

FRANCO-URÍA, A. OTERO-MURAS, I., BALSA-CANTO, E., ALONSO A.A., ROCA E. 2010. Generic parameterization for a pharmacokinetic model to predict Cd concentrations in several tissues of different fish species. *Chemosphere*. 78(4): 377-386

OTERO-MURAS, I. A. FRANCO, A.A. ALONSO, BALSA-CANTO, E. 2010. Dynamic multi-compartmental modelling of metal bioaccumulation in fish: Identifiability implications. *Environmental Modelling & Software*. 25: 344-353

SENDIN, J.O.H., A.A. ALONSO, BANGA, J.R. 2010. Efficient and robust multi-objective optimization of food processing: A novel approach with application to thermal sterilization. *Journal Food Engineering*.98(3): 317-324

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

A. FERNÁNDEZ VILLAVERDE, A. BARREIRO, C. RAIMÚNDEZ. Noviembre 2010. Passive position error correction in Internet-based teleoperation. *Automatica*. 46: 1884-1890

VERA, J., O. RATH, E. BALSACANTO, J. R. BANGA, W. KOLCH AND OLAF WOLKENHAUER. 2010. Investigating dynamics of inhibitory and feedback loops in ERK signalling using power-law models. *Molecular BioSystems* 6(11):2174–2191

RODRIGUEZ-FERNANDEZ, M. AND J.R. BANGA. 2010. SensSB: A software toolbox for the development and sensitivity analysis of systems biology models. *Bioinformatics* 26(13):1675-1676.

SENDIN, J.O.H., O. EXLER & J.R. BANGA. 2010. Multi-objective mixed integer strategy for the optimisation of biological networks. *IET Systems Biology* 4(3):236-248.

EGEA, J.A., MARTÍ, R., & BANGA, J.R. 2010. An evolutionary method for complex-process optimization. *Computers and Operations Research* 37(2):315-324.

J. ROSS, A. FERNÁNDEZ VILLAVERDE. Thermodynamics and Fluctuations far from Equilibrium. Octubre 2010. *Entropy* 12: 2199-2243

BOOKS

GEORGIADIS, MICHAEL C., JULIO R. BANGA AND EFSTRATIOS N. PISTIKOPOULOS .2010. Dynamic process modelling. Wiley-VCH, Weinheim, ISBN-10: 3-527-31684-1

CHAPTERS IN BOOKS

LÓPEZ-QUIROGA E., ANTELO L. T., ALONSO A. A. 2010. Model reduction as a tool for robust predictive control: application to OPR. *20th European Symposium on Computer Aided Chemical Engineering (ESCAPE-20)* - ISBN: 978-0-444-53718-8

ANTELO L. T., FRANCO-URÍA A., ALONSO A. A. 2010. Optimal networking of fishing actor to organise a responsible, optimal and sustainable exploitation of marine resources. *PRES2010 Conference Proceedings*, 4, 1430-1431. ISBN: 978-80-02-02249-7.

ANTELO L. T., BALSACANTO E., TRELEA C., ALONSO, A. A. 2010. Towards efficient operation of freeze-drying processes through real time optimization. *ECCE7 & CHISA2010 Conference Proceedings*. ISBN: 978-80-02-02210-7 (2010).

BALSA-CANTO E., J.R. BANGA AND M.R. GARCÍA 2010. Dynamic Model Building Using Optimal Identification Strategies, with Applications in Bioprocess Engineering. In " Process Systems Engineering Vol. 7 : Dynamic Process Modeling ", Banga J.R., Georgiadis M., Pistikopoulos E. (eds.), Wiley-VCH, Weinheim.

BALSA-CANTO, E., BANGA, J.R. 2010. Computational Procedures for Model Identification. In "Systems Biology for Signaling Networks", Sangdun Choi (Ed.), (pp: 111-138), Springer. ISBN: 978-1-4419-5796-2.

A. A. ALONSO, M. R. GARCIA, C. VILAS 2010. Dynamic Modeling and Simulation for Robust Control of Distributed Processes and Bio-processes. In "Process Systems Engineering Vol. 7 : Dynamic Process Modeling", Banga J.R., Georgiadis M., Pistikopoulos E. (eds.), Wiley-VCH, Weinheim.

Papers in Journals (2005-2009)

2009

EGEA J.A., BALSA-CANTO E., GARCÍA M.R., BANGA J.R. 2009. Dynamic optimization of nonlinear processes with an enhanced scatter search method. *Industrial and Engineering Chemistry Research*, 48(9):4388-4401.

EGEA, J. A., VAZQUEZ, E., BANGA, J. R., MARTÍ, R. 2009. Improved scatter search for the global optimization of computationally expensive dynamic models. *Journal of Global Optimization*, 43(2-3): 175-190.

ESCAÑO, J.M., C. BORDONS, C. VILAS, M.R. GARCIA, ALONSO, A.A. 2009. Neurofuzzy model based predictive control for thermal batch processes. *Journal of Process Control*, 19: 1566-1575

HIRMAJER T., BALSA-CANTO E., BANGA J.R. 2009. DOTcvpSB, a software toolbox for dynamic optimization in systems biology. *BMC Bioinformatics*, 10:199.

KUCHERENKO S., RODRÍGUEZ-FERNÁNDEZ M., PANTELIDES C.C., SHAH N. 2009. Monte Carlo evaluation of Derivative based Global Sensitivity Measures. *Reliability Engineering & System Safety*, 94: 1135-1148.

OTERO-MURAS, I., BANGA, J.R., ALONSO, A.A. 2009. Exploring multiplicity conditions in enzymatic reaction networks. *Biotechnology Progress*, 25(3): 619-631.

OTERO-MURAS I, FRANCO-URÍA A., ALONSO A.A., BALSA-CANTO E. 2009. Dynamic multi compartmental modelling of metal bioaccumulation in fish: Identifiability implications, Environmental Modelling and Software. *Environmental Modelling & Software*, 25(3): 344-353

RODRIGUEZ-FERNANDEZ, M., BANGA, J. R. 2009. Global sensitivity analysis of a biochemical pathway model. *Advances in Soft Computing* 49:233-242

SCHLÜTER, M., ANTELO, L. T., EGEA, J. A., ALONSO, A. A., BANGA, J.R. 2009. An Ant Colony Optimization based algorithm for the integrated process and control system design. *Industrial and Chemistry Engineering Research*, 48(14): 6723-6738.

SCHLÜTER, M., EGEA, J. A., BANGA, J. R. 2009. Extended ant colony optimization for non-convex mixed integer nonlinear programming. *Computers & Operations Research*, 36(7): 2217-2229.

SENDÍN, J.O.H., ALONSO, A. A., BANGA, J. R. 2009. Multi-objective optimization of biological networks for prediction of intracellular fluxes. *Advances in Soft Computing* 49:197-205.

SENDÍN, J. O. H., BANGA, J. R., & CSENDES, T. 2009. Extensions of a multistart clustering algorithm for constrained global optimization problems. *Industrial and Engineering Chemistry Research* 48(6):3014-3023.

2008

ÁLVAREZ-VÁZQUEZ LJ, BALSACANTO E, MARTÍNEZ A. 2008. Optimal design and operation of a wastewater purification system. *Mathematics and Computers in Simulation*, 79 : 668-682.

ANTELO LT, BANGA JR, ALONSO AA. 2008. Hierarchical design of decentralized control structures for the Tennessee-Eastman process. *Computers & Chemical Engineering*, 32: 1995-2015.

ANTELO LT, EXLER O, BANGA JR, ALONSO AA. 2008. Optimal Tuning of Thermodynamic-Based Decentralized PI Control Loops: Application to the Tennessee Eastman Process. *AIChE Journal*, 54 (11): 2904-2924.

BALSACANTO E, ALONSO AA, BANGA JR. 2008. Computational procedures for optimal experimental design in biological systems. *IET Systems Biology*, 2(4): 163-172.

BALSACANTO E, EIFER M, BANGA JR, TIMER J, FLECK C. 2008. Hybrid optimization method with general switching strategy for parameter estimation. *BMC Systems Biology*, 2 (26).

BALSACANTO E, ALONSO AA, BANGA JR. 2008. Computing optimal dynamic experiments for model calibration in predictive microbiology. *Journal of Food Process Engineering*, 31: 186-206.

BANGA JR. 2008. Optimization in computational systems biology. *BMC Systems Biology*, 2: 47.

BANGA JR, BALSACANTO E, ALONSO AA. 2008. Quality and safety models and optimization as part of computer-integrated manufacturing. *Comprehensive Reviews in Food Science and Food Safety*, 7: 168-174.

BANGA JR, BALSACANTO E. 2008. Parameter estimation and optimal experimental design. *Essays in Biochemistry*, 45: 195-209.

CSENDES T, PAL L, SENDIN JOH, BANGA JR. 2008. The GLOBAL Optimization Method Revisited. *Optimization Letters*, 2 (4): 445-454.

EXLER O, ANTELO LT, EGEA JA, ALONSO AA, BANGA, JR. 2008. A tabu search-based algorithm for mixed-integer nonlinear problems and its application to integrated process and control system design. *Computers and Chemical Engineering*, 32: 1877-1891.

GARCÍA MR, VILAS C, BANGA JR, ALONSO AA. 2008. Exponential Observers for Distributed Tubular (Bio)Reactors. *AIChE Journal*, 54 (11): 2943-2956.

IGNATOVA MN, LYUBENOVA VN, GARCÍA MR, VILAS C, ALONSO AA. 2008. Indirect adaptive linearizing control of a class of bioprocesses- Estimator tuning procedure. *Journal of Process Control*, 18 (1): 27-35.

LÓPEZ R, BALSACANTO E, OÑATE E. 2008. Neural networks for variational problems in engineering. *International Journal for Numerical Methods in Engineering*, 75 (11): 1341-1360.

OTERO-MURAS I, SZEDERKÉNYI G, HANGOS KM, ALONSO AA. 2008. Local dissipative Hamiltonian description of reversible reaction networks. *Systems and Control Letters*, 57: 554-560.

OTERO-MURAS I, SZEDERKÉNYI G, HANGOS KM, ALONSO AA. 2008. Dynamic analysis and control of biochemical reaction networks. *Mathematics and Computers in Simulation*, 79: 999-1009.

SCHEERLINCK N, BERHANE NH, MOLES CG, BANGA JR, NICOLAÏ BM. 2008. Optimal dynamic heat generation profiles for simultaneous estimation of thermal food properties using a hotwire probe: computation, implementation and validation. *Journal of Food Engineering*, 84(2): 297-306.

VILAS C, GARCÍA MR, BANGA JR, ALONSO AA. 2008. Desarrollo de una Librería de Componentes en EcosimPro para la Operación de Plantas de Procesamiento Térmico de Alimentos. *Revista Iberoamericana de Automática e Informática Industrial*, 5 (1): 51-65.

VILAS C, GARCÍA MR, BANGA JR, ALONSO AA. 2008. Robust feed-back control of travelling waves in a class of reaction-diffusion distributed biological system. *Physica D: Nonlinear phenomena*, 237 (18): 2353-2364.

2007

ANTELO, LT; OTERO-MURAS, I; BANGA, JR; ALONSO, AA. 2007. A systematic approach to plant-wide control based on thermodynamics. *Computers & Chemical Engineering* 31 (5-6): 677-691.

ANTELO L.T., OTERO-MURAS I., BANGA J.R., ALONSO A.A. 2007. La teoría de redes en ingeniería de control: aplicación al análisis dinámico y al control de procesos. *Revista Iberoamericana de Automática e Informática Industrial*, 4(1): 24-34.

BALSACANTO, E; RODRIGUEZ-FERNANDEZ, M; BANGA, JR. 2007. Optimal design of dynamic experiments for improved estimation of kinetic parameters of thermal degradation. *Journal of Food Engineering* 82 (2): 178-188.

EGEA, JA; RODRIGUEZ-FERNANDEZ, M; BANGA, JR; MARTI, R. 2007. Scatter search for chemical and bio-process optimization. *Journal of Global Optimization* 37 (3): 481-503.

EGEA, J.A., D. VRIES, A.A. ALONSO, J.R. BANGA 2007. Global Optimization for Integrated Design and Control of Computationally Expensive Process Models. *Industrial & Engineering Chemistry Research* 46(26):9148-9157

GARCIA, MR; VILAS, C; BANGA, JR; ALONSO, AA. 2007. Optimal field reconstruction of distributed process systems from partial measurements. *Industrial & Engineering Chemistry Research* 46 (2): 530-539.

RODRIGUEZ-FERNANDEZ, M; BALSACANTO, E; EGEA, JA; BANGA, JR. 2007. Identifiability and robust parameter estimation in food process modeling: Application to a drying model. *Journal of Food Engineering* 83 (3): 374-383.

VERA, J; BALSACANTO, E; WELLSTEAD, P; BANGA, JR; WOLKENHAUER, O. 2007. Power-law models of signal transduction pathways. *Cellular Signalling* 19 (7): 1531-1541.

VILAS, C; GARCIA, MR; BANGA, JR; ALONSO, AA. 2007. Robust feed-back control of distributed chemical reaction systems. *Chemical Engineering Science* 62 (11): 2941-2957.

2006

VILAS, C., GARCÍA, M.R., BANGA, J.R., ALONSO, A.A. 2006 Stabilization of inhomogeneous patterns in a diffusion-reaction system under structural and parametric uncertainties. *Journal of Theoretical Biology* 241(2): 295-306

GARCÍA, M.S.G., BALSACANTO, E., BANGA, J.R., ALONSO, A.A. 2006 Computing optimal operating procedures for the food industry. *Journal of Food Engineering* 74: 13- 23

GARCIA, M. S. G., BALSACANTO, E., VANDE WOUWER, A., BANGA, J. R. 2006 Dynamic Optimization of a Simulated Moving Bed (SMB) Chromatographic Separation Process. *Industrial & Engineering Chemistry Research* 45(26): 9033-9041.

RODRÍGUEZ-FERNÁNDEZ, M., EGEA, J. A., BANGA, J. R. 2006 Novel Metaheuristic for Parameter Estimation in Nonlinear Dynamic Biological Systems. *BMC Bioinformatics* 7: 483

RODRIGUEZ-FERNANDEZ, M., MENDES, P., BANGA, J.R. 2006 A hybrid approach for efficient and robust parameter estimation in biochemical pathways. *BioSystems* 83(2-3): 248-265.

SENDÍN, J.O.H., OTERO, I., ALONSO, A.A., BANGA, J.R. 2006 Improved optimization methods for the multiobjective design of bioprocesses. *Industrial & Engineering Chemistry Research* 45(25): 8594-8603.

SENDIN, O. H., VERA, J., TORRES, N.V., BANGA, J.R. 2006 Model Based Optimization of Biochemical Systems Using Multiple Objectives: A Comparison of Several Solution Strategies. *Mathematical and Computer Modelling of Dynamical Systems* 12 (5): 469-487

2005

Balsa-Canto, E., Alonso, A. A., Banga, J. R. (2005) Dynamic optimization of complex distributed process systems. **Chemical Engineering Research and Design** 83(A8): 1-6.

Banga, J. R., E. Balsa-Canto, C. G. Moles and A. A. Alonso (2005) Dynamic optimization of bioprocesses: Efficient and robust numerical strategies. **Journal of Biotechnology** 117(4):407-419.

Balsa-Canto, E., Vassiliadis, V. S., Banga, J. R. (2005) Dynamic Optimization of Single- and Multi-Stage Systems Using a Hybrid Stochastic-Deterministic Method. **Industrial and Engineering Chemistry Research** 44(5):1514-1523.

COLLABORATIONS

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