

## **RESEARCH PROFILE AND PUBLICATIONS (2005-2015)**

### **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; synthetic biology**)

### **Papers in Journals (2010-2015)**

#### **2015**

ANTELO LT, HIJAS-LISTE GM DE, FRANCO-URÍA A, ALONSO AA, PÉREZ-MARTÍN RI. 2015. Optimisation of processing routes for a marine biorefinery. *Journal of Cleaner Production*, 104: 489-501.

HIJAS-LISTE GM DE, BALSA-CANTO E, EWALD J, BARTL M, LI P, BANGA JR, KALETA C. 2015. Optimal programs of pathway control: dissecting the influence of pathway topology and feedback inhibition on pathway regulation. *BMC Bioinformatics*, 16: 163.

LOPES C, ANTELO LT, FRANCO-URÍA A, ALONSO AA, PÉREZ-MARTÍN RI. 2015. Valorisation of fish by-products against waste management treatments: Comparison of environmental impacts. *Waste Management*, 46: 103-112.

GARCÍA MR, VILAS C, HERRERA JR, BERNÁRDEZ M, BALSACANTO E, ALONSO AA. 2015. Quality and shelf-life prediction for retail fresh hake (*Merluccius merluccius*). *International Journal of Food Microbiology*, 208: 65-74.

VILLAVERDE AF, HENRIQUES D, SMALLBONE K, BONGARD S, SCHMID J, CICIN-SAIN D, CROMBACH A, SAEZ-RODRIGUEZ J, MAUCH K, BALSACANTO E, MENDES P, JAEGER J AND BANGA JR. 2015. BioPreDyn-bench: benchmark problems for kinetic modelling in systems biology. *BMC Systems Biology*, 9(1): 8

VILLAVERDE AF, BONGARD S, MAUCH K, MÜLLER D, BALSACANTO E, SCHMID J, BANGA JR. 2015. A consensus approach for estimating the predictive accuracy of dynamic models in biology. *Computer Methods and Programs in Biomedicine*, 119: 17-28

FOLCH-FORTUNY A, VILLAVERDE AF, FERRER A, BANGA JR. 2015. Enabling network inference methods to handle missing data and outliers. *BMC Bioinformatics*, 16: 283

GABOR A, BANGA JR. 2015. Robust and efficient parameter estimation in dynamic models of biological systems. *BMC Systems Biology*, 9: 74

GABOR A, HANGOS KM, BANGA JR, SZEDERKENYI G. 2015. Reaction Network Realizations of Rational Biochemical Systems and Their Structural Properties. *Journal of Mathematical Chemistry*, 53: 1657-1686.

PÁJARO M, ALONSO AA, VÁZQUEZ C. 2015. Shaping protein distributions in stochastic self-regulated gene expression networks. *Physical Review E*, 92: 032712.

PENAS DR, BANGA JR, GONZÁLEZ P, DOALLO R. 2015. Enhanced parallel Differential Evolution algorithm for problems in computational systems biology. *Applied Soft Computing*, 33: 86-99.

Henriques D, Rocha M, Saez-Rodriguez J, Banga JR. 2015. Reverse engineering of logic-based differential equation models using a mixed-integer dynamic optimization approach. *Bioinformatics*, 31(18): 2999-3007.

PENAS DR, GONZALEZ P, EGEA JA, BANGA JR, DOALLO R. 2015. Parallel Metaheuristics in Computational Biology: An Asynchronous Cooperative Enhanced Scatter Search Method. *Procedia Computer Science*, 51: 630-639

## 2014

I OTERO MURAS, JR BANGA. 2014. Multicriteria global optimization for biocircuit design *BMC Systems Biology*, 8:113.

I OTERO MURAS, P YORDANOV, J STELLING. 2014. A method for inverse bifurcation of biochemical switches: inferring parameters from dose response curves, *BMC Systems Biology*, 8:114.

F LÓPEZ-CAAMAL, DA OYARZÚN, RH MIDDLETON, MR GARCÍA. 2014. Spatial quantification of cytosolic Ca<sup>2+</sup> accumulation in nonexcitable cells: An analytical study. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, 11 (3): 592-603.

A ARIAS-MENDEZ, C VILAS, AA ALONSO, E BALSACANTO. 2014. Time temperature integrators as predictive temperature sensors. *Food Control*, 44: 258-266.

AF VILLAVERDE, JR BANGA. 2014. Reverse engineering and identification in systems biology: strategies, perspectives, and challenges. *Journal of the Royal Society Interface*, 11: 20130505.

C RAIMÚNDEZ, AF VILLAVERDE, A BARREIRO. 2014. Adaptive tracking in mobile robots with input-output linearization. *Journal of Dynamic Systems, Measurement, and Control, Transactions of the ASME*, 136: 054503-1.

AF VILLAVERDE, J ROSS, F MORÁN, JR BANGA. 2014. MIDER: network inference with Mutual Information Distance and Entropy Reduction. *PLOS ONE*, 9(5): e96732.

JA EGEE, D HENRIQUES, T COKELAER, AF VILLAVERDE, A MACNAMARA, D DANCIU, JR BANGA, J SAEZ-RODRIGUEZ. 2014. MEIGO: an open-source software suite based on metaheuristics for global optimization in systems biology and bioinformatics. *BMC Bioinformatics*, 15: 136.

DE HIJAS-LISTE, G.M., E. KLIPP, E. BALSACANTO, J.R. BANGA (2014) Global dynamic optimization approach to predict activation in metabolic pathways. *BMC Systems Biology* 8:1.

HEERMANN, R., K. ZIGANN, S., M. RODRIGUEZ-FERNANDEZ, J.R. BANGA, A. KREMLING, K. JUNG (2014) Dynamics of an Interactive Network Composed of a Bacterial Two-Component System, a Transporter and K<sup>+</sup> as Mediator. *PLoS ONE* 9(2):e89671

T ORDÓÑEZ-DEL PAZO, LT ANTELO, A FRANCO-URÍA, RI PÉREZ-MARTÍN, CG SOTELO, AA ALONSO. 2014. Fish discards management in selected Spanish and Portuguese *métiers*: Identification and potential valorisation. *Trends in Food Science and Technology*, 36 (1), 29-43.

M MOSQUERA-FERNÁNDEZ, P RODRÍGUEZ-LÓPEZ, ML CABO, E BALSACANTO. Numerical spatio-temporal characterization of *Listeria monocytogenes* biofilms. *International Journal of Food Microbiology*, 182, 26-36

A ALONSO, I MOLINA, K THEODOROPOULOS. Modeling bacteria population growth from stochastic single-cell dynamics. *Applied and Environmental Microbiology*, 80 (17), 5241-5253

## 2013

AF VILLAVERDE, J ROSS, JR BANGA. 2013. Reverse engineering cellular networks with information theoretic methods. *Cells*, 2 (2): 306–329.

ALONSO, A.A., ARIAS-MÉNDEZ, A., BALSACANTO, E., GARCÍA, M.R., MOLINA, J.I., VILAS, C., VILLAFÍN, M. 2013. Real time optimization for quality control of batch thermal sterilization of prepackaged foods. *Food Control*, 32 (2): 392-403.

ARIAS-MENDEZ, A., WARNING, A., DATTA, A.K., BALSACANTO, E. 2013. Quality and safety driven optimal operation of deep-fat frying of potato chips. *Journal of Food Engineering*, 119 (1): 125-134.

A ROCHA, JM, GUTIÉRREZ, MJ, ANTELO, LT. 2013. Selectivity, pulse fishing and endogenous lifespan in Beverton-Holt models. *Environmental and Resource Economics*, 54 (1): 139-154.

BECKER, K., E. BALSACANTO, D. CICIN-SAIN, A. HOERMANN, H. JANSSENS, J.R. BANGA, J. JAEGER. 2013. Reverse-Engineering Post-Transcriptional Regulation of Gap Genes in *Drosophila melanogaster*. *PLoS Computational Biology*, 9 (10): e1003281.

EGEA, J.A., D. HENRIQUES, T. COKELAER, A.F. VILLAVARDE, J.R. BANGA, J. SAEZ-RODRIGUEZ. 2013. MEIGO: an open-source software suite based on metaheuristics for global optimization in systems biology and bioinformatics. *arXiv:1311.5735*.

LOPES, C, ANTELO, LT, FRANCO-URÍA, A, BOTANA, C, ALONSO, AA. 2013. Sustainability of port activities within the framework of the fisheries sector: Port of Vigo (NW Spain). *Ecological Indicators*, 30: 45-51.

R. HANNEMANN-TAMÁS, A. GÁBOR, SZEDERKÉNYI G, K. M. HANGOS. 2013. Model complexity reduction of chemical reaction networks using mixed-integer quadratic programming. *Computers and Mathematics with Applications*, 65 (10): 1575-1595.

RIVAS D, VILAS C, VARAS F, ALONSO AA. 2013. Derivation of postharvest fruit behavior reduced order models for on-line monitoring and control of quality parameters during refrigeration. *Journal of food process engineering*, 36 (4): 480-491.

RODRIGUEZ-FERNANDEZ, M., M. REHBERG, A. KREMLING, J.R. BANGA. 2013. Simultaneous model discrimination and parameter estimation in dynamic models of cellular systems. *BMC Systems Biology*, 7: 76.

TUZA, Z.A., G. SZEDERKENYI, K.M. HANGOS, A.A. ALONSO, J.R. BANGA. 2013. Computing all Sparse Kinetic Structures for a Lorenz System Using Optimization. *Int. Journal of Bifurcation and Chaos*, 23 (8): 1350141.

## **2012**

ANTELO LT, LOPES C, FRANCO-URÍA A, ALONSO AA. 2012. Fish discards management: Pollution levels and best available removal techniques. *Marine Pollution Bulletin*, 64 (7): 1277-1290.

ANTELO LT, PASSOT S, FONSECA F, TRELEA IC, ALONSO AA. 2012. Towards optimal operation conditions of freeze-drying processes via a multi-level approach. *Drying Technology*, 30 (13): 1432-1448.

BALSACANTO E, BANGA JR, EGEA JA, VILLAVARDE AF, DE HIJAS-LISTE GM. 2012. Global optimization in systems biology: stochastic methods and their applications. *Advances in Experimental Medicine and Biology*, 736: 409-425.

GARCÍA MR, VILAS C, SANTOS LO, ALONSO AA. 2012. A robust multi-model predictive controller for distributed parameter systems. *Journal of Process Control*, 22-1: 60-71.

- HIGUERA C, VILLAVERDE AF, BANGA JR, ROSS J, MORÁN F. 2012. Multi-criteria optimization of regulation in metabolic networks. *PLoS ONE*, 7 (7): e41122.
- LOPES C, HERVA M, FRANCO-URÍA A, ROCA E. 2012. Multicorrelation models and uptake factors to estimate extractable metal concentrations from soil and metal in plants in pasturelands fertilized with manure. *Environmental Pollution*, 166: 17-22.
- LÓPEZ-QUIROGA E, ANTELO LT, ALONSO AA. 2012. Time-scale modeling and optimal control of freeze-drying. *Journal of Food Engineering*, 111 (4): 655-666.
- MACNAMARA A, TERFVE C, HENRIQUES D, BERNABÉ BP, SAEZ-RODRIGUEZ J. 2012. State-time spectrum of signal transduction logic models. *Physical biology*, 9: 16pp.
- MARTÍN E, MEIS M, MOURENZA C, RIVAS D, VARAS F. 2012. Fast solution of direct and inverse design problems concerning furnace operation conditions in steel industry. *Applied Thermal Engineering*, 47: 41-53.
- OTERO-MURAS I, BANGA JR, ALONSO AA. 2012. Characterizing multistationarity regimes in biochemical reaction networks. *PLoS ONE*, 7 (7): e39194.
- RAIMÚNDEZ C, BARREIRO A, VILLAVERDE AF, 2012. Damping injection by reset control. *Journal of Dynamic Systems, Measurement, and Control*, 134 (2): 024504.
- ROCHA JM, GUTIERREZ MJ, ANTELO LT. 2012. Pulse Vs. Optimal Stationary Fishing: The Northern Stock of Hake. *Fisheries Research*, 121-122: 51-62.
- ROCHA JM, GUTIERREZ MJ, ANTELO LT. 2012. Selectivity, Pulse Fishing and Endogenous Lifespan in Beverton-Holt Models. *Environmental and Resource Economics*. In press, 10. 1007/s10640-012-9.
- ROCHA JM, GUTIERREZ MJ, CERVIÑO S, ANTELO LT. 2012. "logMSY" and optimal harvesting control rules: New tools for the implementation. *Ocean and Coastal Management*, 70: 48-53.
- RODRÍGUEZ-FERNÁNDEZ M, BANGA JR, DOYLE FJ. 2012. Novel global sensitivity and analysis methodology accounting for the crucial role of the distribution of input parameters: application to systems biology models. *Int. J. of Robust and Nonlinear Control*, 22 (10): 1082-1102.
- SZEDERKENYI G, BANGA JR, ALONSO AA. 2012. CRNreals: a toolbox for distinguishability and identifiability analysis of biochemical reaction networks. *Bioinformatics*, 28 (11): 1549-1550.
- TERFVE C, COKELAER T, HENRIQUES D, MACNAMARA A, GONÇALVES E, MORRIS MK, VAN IERSEL M, LAUFFERNGURGER DA, SAEZ-RODRIGUEZ J. 2012. CellNOptR: a flexible toolkit to train protein signalling networks to data using multiple logic formalisms. *BMC systems biology*, 6: 16pp.
- VILAS C, BALSACANTO E, GARCÍA S, BANGA JR, ALONSO AA. 2012. Dynamic optimization of distributed biological systems using robust and efficient numerical techniques. *BMC systems biology*, 6: 79.
- VILLAVERDE AF, EGEE JA, BANGA JR. 2012. A cooperative strategy for parameter estimation in large scale systems biology models. *BMC Systems Biology*, 6: 75.

VILLAVERDE AF, RAIMÚNDEZ C, BARREIRO A. 2012. Passive internet-based crane teleoperation with haptic aids. *International Journal of Control, Automation and Systems*, 10 (1): 78-87.

## 2011

BALSA-CANTO E, BANGA J R. 2011. AMIGO, a toolbox for Advanced Model Identification in systems biology using Global Optimization. *Bioinformatics*, 27(16):2311-2313.

CHIS O, BANGA J R, BALSA-CANTO E. 2011. GenSSI: a software toolbox for structural identifiability analysis of biological models. *Bioinformatics*, 27 (18): 2610- 2611.

CHIS O, BANGA J R, BALSA-CANTO E. 2011. Structural Identifiability of Systems Biology Models: A Critical Comparison of Methods. *PLoS ONE*, 6 (11): e27755.

CHIS O, NEAMTU M, OPRIS D. 2011. Deterministic and Stochastic Model for the Role of the Immune Response Time Delay in Periodic Therapy of the Tumors. *Current Computer-Aided Drug Design*, 7: 338-350.

CHIS O, OPRIS D. 2011. Generalized fractional hybrid Hamilton–Pontryagin equations. *International Journal of Geometric Methods in Modern Physics (IJGMMP)*, 8: 245-264.

FERNÁNDEZ A, BLAS A, TORRICO A, CARRASCO J. 2011. Reset control for passive bilateral teleoperation. *IEEE Transactions on Industrial Electronics*, 58: 3037-3045.

FERNÁNDEZ A, ROSS J, MORÁN F, BALSA-CANTO E, BANGA J R. 2011. Use of a generalized Fisher equatic for global optimization in chemical kinetics. *Journal of Physical Chemistry A*, 115 (30): 8426-8436.

GÁBOR A, FAZEKAS C, SZEDERKÉNYI G, HANGOS K M. 2011. Modeling and Identification of a Nuclear Reactor with Temperature Effects and Xenon Positioning. *European Journal of Control*, 17 (1): 104-115.

GARCÍA M R, VILAS C, BALSA-CANTO E, LYUBENOVAC V, IGNATOVAC M N, ALONSO A A. 2011. On-line estimation in a distributed parameter bioreactor: Application to the gluconic acid production. *Computers and Chemical Engineering*, 35(1):84-91.

GARCÍA M R, VILAS C, SANTOS L O, ALONSO A A. 2011. A robust multi-model predictive controller for distributed parameter systems. *Journal of Process Control A*, In press doi: 10.1016/j.jprocont.2011.10.008.

KOTHARE M V, BANGA J R. 2011. Editorial - DYCOPS and CAB Special Issue. *Journal of Process Control*, 21(10): 1359-1360.

NICOLAÏ B M, EGEA J A, SCHEERLINCK N, BANGA J R. 2011. Fuzzy finite element analysis of heat conduction problems with uncertain parameters. *Journal of Food Engineering*, 103(1): 38-46.

RODRIGUEZ-FERNANDEZ M, CARDELLE-COBAS A, VILLAMIEL M, BANGA, J R. 2011. Detailed kinetic model describing new oligosaccharides synthesis using different  $\beta$ -galactosidases. *Journal of Biotechnology*, 153(3-4): 116-124.

SYAFIIE S, TADEO S, VILLAFIN, M, ALONSO A A. 2011. Learning control for batch thermal sterilization of canned foods. *ISA Transactions*, 50 (1): 82-90.

SZEDERKENYI G, BANGA J R, ALONSO A A. 2011. Inference of complex biological networks: distinguishability issues and optimization-based solutions. *BMC Systems Biology*, 5:177.

SZEDERKÉNYI G, HANGOS K M. 2011. Finding complex balanced and detailed balanced realizations of chemical reaction networks. *Journal of Mathematical Chemistry*, 49 (6): 1163-1179.

SZEDERKÉNYI G, HANGOS K M. 2011. Mass action realizations of reaction kinetic system models on various time scales. *Journal of Physics – Conference Series*, 268 (1): 012009.

SZEDERKÉNYI G, HANGOS K M, PÉNI T. 2011. Maximal and Minimal Realizations of Reaction Kinetic Systems: Computation and Properties. *Match – Communications in Mathematical and in Computer Chemistry*, 65 (2): 177.

## Papers in Journals (2005-2010)

### 2010

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

VERA, J., O. RATH, E. BALSA-CANTO, 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. *20<sup>th</sup> 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).

BALSACANTO 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.

BALSACANTO, 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.

## 2009



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

BALSA-CANTO, 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; EGEEA, 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.

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