

Papers on MODELING and SIMULATION by PSE-Lab

CMIC Department – Politecnico di Milano

davide.manca@polimi.it

Keywords: Modeling; Simulation; Steady-state models; Dynamic models; First principle models; Black-box models; Artificial Neural Networks (ANN); Numerical models; Case studies; Distillation systems; Batch distillation; Incineration plant; Combustion processes; Drug delivery systems; Reverse reactors; Simulated moving bed reactors (SMBR); Reverse osmosis; Accident simulation; Event reconstruction; Industrial accidents; BP Texas City accident; Viareggio accident.

- (2) **RIGOROUS DYNAMIC MODELLING AND CONTROL SYSTEM SYNTHESIS FOR DISTILLATION PROCESSES: AN INTEGRATED APPROACH**
M. Rovaglio, T. Faravelli, G. Biardi, M. Banfi, D. Manca
Proceedings of "ComChem: Computer Applications in Chemical Engineering", The Hague, The Netherlands, pp. 133-138, (1990)
- (5) **DYCODIS: A SIMULATION PACKAGE FOR RIGOROUS DYNAMICS NONLINEAR CONTROL OF DISTILLATION SYSTEMS**
M. Rovaglio, T. Faravelli, D. Manca
Proceedings of "ESM: European Simulation Multiconference", pp. 827-833, Copenhagen Denmark, (1991)
- (6) **CRUDE OIL CHARACTERIZATION FOR TOPPING UNITS OPTIMIZATION**
D. Manca
Chemical Engineering Forum for Young Scientists, Torino 2-4 July, (1992)
- (9) **STATE OF THE ART AND RESEARCH TRENDS IN CHEMICAL ENGINEERING SIMULATION**
G. Biardi, D. Manca, M. Rovaglio
"International Conference on High Performance Computing in Manufacturing and Process Simulation", Roma, 18-20 October, (1993)
- (10) **DYNAMIC MODELING OF WASTE INCINERATION SYSTEMS: A STARTUP PROCEDURE**
M. Rovaglio, D. Manca, G. Biardi, J. Falcon
Comp. Chem. Engng., Vol. 18, S361-S368, (1994)
[http://dx.doi.org/10.1016/0098-1354\(94\)80060-X](http://dx.doi.org/10.1016/0098-1354(94)80060-X)
- (31) **DYNAMIC MODELING OF WASTE INCINERATION PLANTS WITH ROTARY KILNS: COMPARISONS BETWEEN EXPERIMENTAL AND SIMULATION DATA**
M. Rovaglio, D. Manca, G. Biardi
Chemical Engineering Science, Vol. 53, No. 15, pp. 2727-2742, (1998)
[http://dx.doi.org/10.1016/S0009-2509\(98\)00081-5](http://dx.doi.org/10.1016/S0009-2509(98)00081-5)
- (52) **COMPLEX DYNAMIC BEHAVIOUR IN THE RING REACTOR FOR METHANOL SYNTHESIS**
S. Velardi, A. Barresi, D. Manca, D. Fissore
Proceedings of Dinip 2002, I.III, Benevento, April 11-13, (2002)
- (53) **DYNAMIC ANALYSIS OF DISCONTINUOUS INCINERATION PROCESSES**
D. Manca, E. Mancusi
Proceedings of Dinip 2002, IV.I, Benevento, April 11-13, (2002)

- (55) **A GENERALISED PROGRAM FOR FUEL CELL SYSTEMS SIMULATION**
S. Pierucci, D. Manca, S. Galli, M. Mangione
Proceedings of ESCAPE-12, The Hague, May 26-29, 307-312, (2002)
[http://dx.doi.org/10.1016/S1570-7946\(02\)80079-7](http://dx.doi.org/10.1016/S1570-7946(02)80079-7)
- (57) **MODELING THE CONTROLLED RELEASE OF MICROENCAPSULATED DRUGS: THEORY AND EXPERIMENTAL VALIDATION**
D. Manca, M. Rovaglio
Chemical Engineering Science, **58**, Issue 7, 1337-1351, (2003)
[http://dx.doi.org/10.1016/S0009-2509\(02\)00623-1](http://dx.doi.org/10.1016/S0009-2509(02)00623-1)
- (59) **MODELING THE POLYMER COATING IN MICROENCAPSULATED ACTIVE PRINCIPLES**
D. Manca, M. Rovaglio, I. Colombo
Proceedings of ESCAPE-13, 1115-1120, Elsevier, ISBN 0-444-51368-X, (2003)
[http://dx.doi.org/10.1016/S1570-7946\(03\)80267-5](http://dx.doi.org/10.1016/S1570-7946(03)80267-5)
- (62) **MATHEMATICAL MODELLING OF THE EVAPORATION AND COMBUSTION OF SINGLE N-HEPTANE DROPLETS UNDER MICROGRAVITY CONDITIONS**
S. Corno, M. Perego, G. Buzzi Ferraris, T. Faravelli, D. Manca, E. Ranzi and T. Parra
ICE 2003 6th International Conference on Engines for Automobile, Capri September 14-19, (2003)
- (63) **COMPLEX DYNAMIC BEHAVIOUR OF METHANOL SYNTHESIS IN THE RING REACTOR NETWORK**
S. Velardi, A. Barresi, D. Manca, D. Fissore
Chemical Engineering Journal, **99**, 117-123, (2004)
<http://dx.doi.org/10.1016/j.cej.2003.09.008>
- (66) **BURNING RATES AND SOOT PROPENSITY OF ISOLATED ETHANOL FUEL DROPLETS IN MICROGRAVITY CONDITIONS**
M. Mehl, M. Perego, D. Manca, T. Faravelli, E. Ranzi
Proceedings of the Joint Meeting of Greek and Italian Sections of the Combustion Institute, Corfù, P63.1-P63.4, (2004)
- (67) **DYNAMIC MODELING OF A POLY(ETHYLENE TEREPHTHALATE) SOLID-STATE POLYMERIZATION REACTOR II: MODEL PREDICTIVE CONTROL**
M. Rovaglio, C. Algeri, and D. Manca
Ind. Eng. Chem. Res., **43**, 4267-4277, (2004)
- (68) **MODELLING OF METHANOL SYNTHESIS IN A NETWORK OF FORCED UNSTEADY-STATE RING REACTORS BY ARTIFICIAL NEURAL NETWORKS FOR CONTROL PURPOSES**
D. Fissore, A. A. Barresi, D. Manca
Chem. Eng. Sci., **59**, 4033 – 4041, (2004)
<http://dx.doi.org/10.1016/j.ces.2004.05.033>
- (69) **IMPACTS ASSESSMENT AND TRADE-OFFS OF FUEL CELL BASED APUS**
F. Baratto, U. M. Diwekar, G. Buzzi Ferraris, D. Manca
Chem. Eng. Trans., **4**, 385-390, ISBN 88-900775-3-0, (2004)
- (76) **IMPACTS ASSESSMENT AND TRADE-OFFS OF FUEL CELL-BASED AUXILIARY POWER UNITS PART I: SYSTEM PERFORMANCE AND COST MODELING**
F. Baratto, U. M. Diwekar, D. Manca
Journal of Power Sources, **139**, 205-213, (2005)
<http://dx.doi.org/10.1016/j.jpowsour.2004.07.023>
- (77) **IMPACTS ASSESSMENT AND TRADEOFFS OF FUEL CELL BASED AUXILIARY POWER UNITS PART II. ENVIRONMENTAL AND HEALTH IMPACTS, LCA, AND MULTI-OBJECTIVE OPTIMIZATION**
F. Baratto, U. M. Diwekar, D. Manca
Journal of Power Sources, **139**, 214-222, (2005)
<http://dx.doi.org/10.1016/j.jpowsour.2004.07.024>

- (78) **NUMERICAL MODELING OF A DISCONTINUOUS INCINERATION PROCESS WITH ON-LINE VALIDATION**
D. Manca, M. Rovaglio
Ind. Eng. Chem. Res., 44, 3159-3177, (2005)
<http://dx.doi.org/10.1021/ie0495473>
- (99) **ADVANCES IN PLANT-WIDE DESIGN AND CONTROL BY PROCESS DYNAMIC SIMULATION**
F. Manenti, D. Manca
Second place winner "Excellence in Simulation", University Grant Program Simsci-Esscor (Invensys Process Systems), 23-40, Ed. C. Hastings, Lake Forest, CA, USA, (2007)
- (101) **ON POOL SPREADING AROUND TANKS: GEOMETRICAL CONSIDERATIONS**
S. Brambilla, D. Manca
Journal of Hazardous Materials, **158**, 88-99, (2008)
<http://dx.doi.org/10.1016/j.jhazmat.2008.01.049>
- (107) **CHALLENGES IN INDUSTRIAL DYNAMICS: COUPLING PROCESS SIMULATION WITH ACCIDENT SIMULATION**
S. Brambilla, D. Manca
PSAM-9 International Conference on Probabilistic Safety Assessment and Management, Hong Kong 18-23 May, **422**, 1-5, (2008)
- (112) **PROCESS DYNAMIC AND INDUSTRIAL ACCIDENT SIMULATORS: COUPLING TWO DIFFERENT WORLDS INTO AN INTEGRATED PLATFORM**
S. Brambilla, F. Manenti, D. Manca
Proceedings of ESCAPE-18, P217, 1-6, Elsevier, ISBN 978-0-444-53228-2, Editors B. Braunschweig and X. Joulia, (2008)
- (123) **MOLECULAR DISTILLATION. MODELING AND SIMULATION TO SPLIT HEAVY PETROLEUM FRACTIONS**
L. Zuniga, N. M. Nascimento Lima, M. R. Wolf Maciel, R. Maciel Filho, C. B. Batistella, D. Manca, F. Manenti, L. C. Medina
Proceedings of AIChE Meeting. Colorado, USA, 1-11, (2008)
- (124) **ACCIDENTS INVOLVING LIQUIDS: A STEP AHEAD IN MODELING POOL SPREADING, EVAPORATION AND BURNING**
Sara Brambilla, Davide Manca
Journal of Hazardous Materials, **161**, 1265-1280, (2009)
<http://dx.doi.org/10.1016/j.jhazmat.2008.04.109>
- (127) **DYNAMIC PROCESS AND ACCIDENT SIMULATIONS AS TOOLS TO PREVENT INDUSTRIAL ACCIDENTS**
Sara Brambilla, Davide Manca
Chemical Product and Process Modeling: Vol. 4: 2, 1-20, (2009)
<http://dx.doi.org/10.2202/1934-2659.1295>
- (130) **DYNAMIC SIMULATION OF INDUSTRIAL ACCIDENTS**
Davide Manca, Sara Brambilla
Chemical Engineering Transactions, **17**, 299-304, (2009)
<http://dx.doi.org/10.3303/CET0917051>
- (133) **MODELING AND SIMULATION OF MOLECULAR DISTILLATION PROCESS FOR A HEAVY PETROLEUM CUT**
L.L. Zuñiga, N.M.N. Lima, M.R. Wolf Maciel, R. Maciel Filho, C.B. Batistella, D. Manca, F. Manenti, L.C. Medina
Chemical Engineering Transactions, **17**, 1639-1644, (2009)
<http://dx.doi.org/10.3303/CET0917274>
- (138) **DYNAMIC SIMULATION OF INDUSTRIAL ACCIDENTS**
Davide Manca, Sara Brambilla
ACS, Vol. 9, 197-204, ISBN 978-88-95608-10-5, ISSN 2036-5969, Reed Business Information, Milan, (2009)

- (140) **SIMULATION OF THE LPG RELEASE, DISPERSION, AND EXPLOSION IN THE VIAREGGIO RAILWAY ACCIDENT**
S. Brambilla, R. Totaro, D. Manca
Chemical Engineering Transactions, **19**, 195-200, (2010)
<http://dx.doi.org/10.3303/CET1019032>
- (142) **THE VIAREGGIO LPG RAILWAY ACCIDENT: EVENT RECONSTRUCTION AND MODELING**
S. Brambilla, D. Manca
Journal of Hazardous Materials, **182**, 346-357, (2010)
<http://dx.doi.org/10.1016/j.jhazmat.2010.06.039>
- (150) **INCREASING THE UNDERSTANDING OF THE BP TEXAS CITY REFINERY ACCIDENT**
D. Manca, S. Brambilla, A. Villa
Computer Aided Chemical Engineering, Volume 29, Pages 1266-1270, (2011)
<http://dx.doi.org/10.1016/B978-0-444-54298-4.50032-5>
- (171) **DYNAMIC SIMULATION OF THE BP TEXAS CITY REFINERY ACCIDENT**
D. Manca, S. Brambilla
Journal of Loss Prevention in the Process Industries, **25**, 6, 950-957, (2012)
<http://dx.doi.org/10.1016/j.jlp.2012.05.008>
- (173) **A PLANT SIMULATOR TO ENHANCE THE PROCESS SAFETY OF INDUSTRIAL OPERATORS**
D. Manca, S. Colombo, S. Nazir
SPE European HSE Conference and Exhibition 2013: Health, Safety, Environment and Social Responsibility in the Oil and Gas Exploration and Production Industry; London; United Kingdom; 16 April 2013 through 18 April 2013; Code 98713, ISBN 978-162748284-4, 394-404, (2013)
<http://dx.doi.org/10.2118/164992-MS>
- (176) **MODELING THE COMMODITY FLUCTUATIONS OF OPEX TERMS**
D. Manca
Computers and Chemical Engineering, **57**, 3-9, (2013)
<http://dx.doi.org/10.1016/j.compchemeng.2013.04.018>
- (178) **A METHODOLOGY TO FORECAST THE PRICE OF ELECTRIC ENERGY**
D. Manca
Computer Aided Chemical Engineering, **32**, 679-684, (2013)
<http://dx.doi.org/10.1016/B978-0-444-63234-0.50114-7>
- (183) **NEURAL NETWORK BASED CORRELATION FOR ESTIMATING WATER PERMEABILITY CONSTANT IN RO DESALINATION PROCESS UNDER FOULING**
M. Barello, D. Manca, R. Patel, I.M. Mujtaba
Desalination, **345**, 101-111, (2014)
<http://dx.doi.org/10.1016/j.desal.2014.04.016>
- (190) **OPERATION AND MODELING OF RO DESALINATION PROCESS IN BATCH MODE**
M. Barello, D. Manca, R. Patel, I.M. Mujtaba
Computer Aided Chemical Engineering, **33**, 451-456, (2014)
<http://dx.doi.org/10.1016/B978-0-444-63456-6.50076-4>
- (191) **STOCHASTIC PRICE/COST MODELS FOR SUPPLY CHAIN MANAGEMENT OF REFINERIES**
R. Rasello, D. Manca
Computer Aided Chemical Engineering, **33**, 433-438, (2014)
<http://dx.doi.org/10.1016/B978-0-444-63456-6.50073-9>
- (195) **NEURAL NETWORK BASED CORRELATION FOR ESTIMATING WATER PERMEABILITY CONSTANT IN RO DESALINATION PROCESS UNDER FOULING**
M. Barello, D. Manca, R. Patel, I.M. Mujtaba
Desalination, **345**, 101-111, (2014)
<http://dx.doi.org/10.1016/j.desal.2014.04.016>