Chapter 7

Final Comments and Conclusions

Ars longa, vita brevis

7.1 Thesis contribution

The main contributions of this thesis are summarised next. At the **analysis** stage of the work a set of issues have emerged:

- Although the implementation of the on-line optimisation technology appears to lead to significant economical improvements, it has not the wide acceptance one may expect. This fact is clearly verified observing the number of on-line optimisation applications as compared to that of advanced process control.

- Industrial practitioners have pointed out concrete weak points, like the undesired steady state wait, optimisation robustness and maintenance aspects. Nevertheless, academic research has focused in particular points of the on-line optimisation loop without satisfactory answers to those points.

- There has not been a change in the on-line optimisation strategy since the first implementation of the RTO technology.[1]

- There is a lack of systematic procedure for implementing the discrete decision involved in the optimisation of continuous process with decaying performance.

Such observations have inspired a deep for review of the strategy conducted by an on-line optimisation system. It has been considered that the factors motivating an on-line decision making problem comes from disturbances occurrence. The combined effect of both internal and external

[1] There have been several proposals for performing some functionalities simultaneously, as for instance data reconciliation and parameter estimation. However, these topics have nothing to do with the *operation optimisation* strategy.

disturbances leads to an (hypothetical) moving optimum. Furthermore, when internal disturbances are related to process degradation, a maintenance problems arise. Consequently, two procedures have resulted at the **synthesis** stage to deal with such situations:

- Real Time Evolution (RTE) has been developed as an alternative to classical RTO systems with the aim of tracking such moving optimum.

  1. The RTE system produces a successive improvement of plant performance, making the plant evolve continuously toward the objectives without performing formal optimisation (as explained, in that context, the concept of optimum is quite weak).
  2. The procedure is based in main (external) disturbance measurements and a steady state model.
  3. Although RTE requires more time than RTO to reach optimum operating conditions, it improves plant performance immediately after disturbances occur, thus resulting in an overall faster and smoother system, which is able to deal even with continuous changes.
  4. The algorithms involved in RTE (improvement) are simpler and faster than those used by RTO (optimisation); this allows the intensive use of the available rigorous process model with little computational effort.
  5. Since the solution for stocastics problems becomes substantially simplified, a way for dealing with uncertainty have been also proposed (Robust RTE).
  6. Results show that the RTE strategy appears less affected than RTO when using a poor controller performance.

- Regarding internal disturbances and the associated discrete decisions involved in operation shut down, a step forward towards the integration of classical mathematical formulations for the maintenance planning of processes with decaying performance and on-line optimisation have resulted, as an extention of the previous RTE strategy.

  1. A way for the off-line calculation of a maintenance plan and a methodology for the on-line implementation of such planed decisions in a co-ordinated way have been developed.
  2. A simple and general NLP formulation of the problem has been proposed, involving general performance relationships and mass balances, which allows its use over a wide range of applications. The variables involved have a clear physical meaning, and the computation times required are indeed affordable. The solutions are easy to implement, and even more, they can be further used for performing on-line optimisation.
  3. The proposed procedure for on-line optimisation is quite simple, robust and reduces the effects of plant model mismatch and variability. It is based in the previously

mentioned formulation, and an ulterior transformation of the problem to solve it on-line, using a reduced space that only includes operating times as decision variables.

4. In order to properly evaluate the degradation status of the plant, the strategy uses measurements about the system outputs rather than inputs. This RTE strategy has proved to obtain good solutions by using properly the information coming from the plant and answering simple questions on line, rather than performing successive formal optimisation, which has been the commonly used strategy.

5. The on-line procedure seems to be especially worthwhile in cases with highly decreasing performance rates and where the off-line optimal solution is not strongly dictated by the constraints.

It is important to note, that both approaches may be coordinately applied when both, external and internal disturbances occur, as has been illustrated.

With purposes of **validation** of the proposed methodologies, well known benchmarks have been used. Thus, although the obtained results are encouraging, a categoric generalisation is not possible. Nevertheless, a careful qualitative analisys of the considered problems allows to extrapolate the main observations to other scenarios without significant loss of accuracy. Furthermore, the strategies have proved very satisfactory results when applied to **industrial problems**. Not only they are perfectly applicable, but also, they have shown again to have in favour many advantages as compared to other approaches. It is also important to mention that the fact of validating the approaches have proved to be a mean for increasing benefits and gaining better understanding of the process, its associated trade-offs and greatly helping to proper bottleneck identification.

Since this thesis corresponds to the applied sciences research field some **implementation related issues** have been considered.[2]Aspects about the way the process dynamics influence the RTE design have been considered, with the aim of providing a method for a proper RTE parameters tuning. Indeed, a way for on-line tuning has been also suggested (Adaptive RTE). The influence of the control system quality has not been neglected and some insight has been given from two points of view: the economical performance and the operational one. Finally, modular software design aspects have been also tackled even for the simple prototypes used during this thesis work, with the aim of setting some guidelines for industrial implementation.

[2]This aspect have been of major importance for a Spanish research project strongly linked to this thesis work: REALISSTICO (CICYT, QUI-99-1091).

Nomenclature

Acronyms

ARTE: Adaptative Real Time Evolution.

CAPE: Computer Aided Process Engineering.

CLRTO: Closed Loop Real Time Optimisation.

CO: Cape-Open.

COM: Component Object Model.

DAE: differential and algebraic equation.

DCS: Distributed Control System.

DDE: Dynamic Data Exchange.

DM: Data Manager.

DR: Data Reconciliation.

GED: Gross Error Detection.

GRG: Generalised Reduced Gradient.

GUI: Graphical User Interface.

LP: Linear Programming.

MILP: Mixed Integer-Linear Programming.

MINLP: Mixed Integer-Non-Linear Programming.

MPC: Model Predictive Control.

MU: Model Updating.

NLP: Non-Linear Programming.

PE: Parameter Estimation.

PEDR: Parameter Estimation and Data Reconciliation.

PID: Proportional-Integer-Derivative controller.

PSS: Pseudo Steady State.

QP: Quadratic Programming.

RRTE: Robust Real Time Evolution.

RTE: Real Time Evolution.

RTO: Real Time Optimisation.

SFC: Sequential Function Charts.

SLP: Successive Linear Programming.

SPC: Statistical Process Control.

SQP: Successive Quadratic Programming.

SS: Steady State.

SSID: Steady State Identification.

VBA: Visual Basic for Applications.

Notation

A: evaporator heat exchange area.

A_p: section perpendicular to the flow.

a: parameter adjusted experimentally.

b: parameter adjusted experimentally.

C: cooling costs.

C_f: filtration capacity.

C_m: maintenance cost.

c: parameter adjusted experimentally.

c_q: economical weighting factor for cooling streams.

$D(s)$: disturbances in the Laplace domain.

d_p: equivalent diameter of the particles in the filtration cake.

F_i: mass flow of i.

$F_k[\cdot]$: non linear operator that denotes the set of differentials equations associated to the state k.

F_r^{bias}: bias used in the reactor volume controller.

f: process model.

F_m: average feed rate during the whole cycle.

f_p: friction factor.

fq: quality coefficient.

$G_P(s)$: process transfer function.

$G_C(s)$: controller transfer function.

$G_{SP}(s)$: transfer function of the closed loop system with respect to the set-point.

$G_{DC}(s)$: transfer function of the closed loop system with respect to the disturbance.

g: operational constraints.

H: heating costs.

h_f: pressure drop associated to friction losses.

h_q: economical weighting factor for heating streams.

$INVNS$: inverse of the normal standard cumulative distribution.

IOF: Instantaneous Objective Function.

$\overline{IOF}$: mean value of the Instantaneous Objective Function frequency distribution.

k: auxiliary integer variable denoting discrete intervals.

$k_{()}$: kinetic coefficient for the reaction $()$.

k_p^c: proportional effect parameter of a controller.

L: length of the cake (depth).

$L_{kk'}$: scalar boolean function which determines when a transition between the states k and k' is triggered.

MOF: Mean Objective Function.

MOF_∞: MOF value when the time tends to infinity (for a sinusoidal disturbance).

M: mass.

MX: sugar mass.

N: a big integer number.

n: number of sub-cycles during the total cycle time.

OF: generic objective function.

P: price parameter.

p: given parameters (a disturbance belongs to this set).

Pf: fractional production associated to a line.

Pf': fraction of product produced a line, corrected by a factor to include the non-productive part.

$Q_{()}$: energy associated to the stream $()$.

q: rational number.

qf: quality index.

R: revenues obtained for selling the products.

RM: raw material costs.

Re_p: Reynolds' number for fluid flow through packed beds.

R_m: filtration medium resistance.

r: economic conversion factor.

r_m: economical weighting factor for raw material streams.

$rand$: uniformly distributed random number.

$\mathbf{S}_k$: discrete state k.

Sf: split fraction.

Sf_E: extracted split fraction.

S_t: process settling time.

$SP(s)$: set-points in the Laplace domain.

s: system state variable.

s: Laplace domain variable.

T: temperature.

Tf: time fraction a given unit devoted to process with a given feed.

T_{cycle}: total cycle duration.

T_r^{sp}: set-point for the reactor temperature.

T_i^c: integral effect parameter.

$\mathbf{T}_{kk'}$: set of possible transitions between the pair of states (k, k').

t: total processing time.

t_0: reference time.

ts: operating time for a sub-cycle.

U: heat exchange coefficient.

V: filtered volume.

V_e: equivalent filtered volume for the filtration media.

V_r^{pv}: reactor volume (process variable).

V_r^{sp}: reactor volume (set-point).

w: weight coefficient for the pair quality-factor-product.

X: mass fraction.

x: free operational variable.

Y: conversion.

y: system output variable.

$y(s)$: system output in the Laplace domain.

Z: total profit.

Sub indexes

c: cooling.

$current$: current value.

end: final value.

h: heating.

i: element in a set, commonly refers a material.

ini: initial value.

j: element in a set, commonly refers a unit.

k: element in a set, commonly refers an interval or a possible state.

lo: lower bound.

m: element in a set of a reduced space of feeds.

n: element in a set of a reduced space of units.

nom: nominal value.

opt: optimal value.

p: product.

r: reactor.

rm: raw material.

ss: steady state value.

up: upper bound.

T: total.

α: fixed parameter.

β: parameter updated on-line.

γ: economical parameter.

π: internal disturbance parameter.

Greek Letters

α:	specific cake resistance.
β:	auxiliary coefficient to characterise an evaporation effect.
β_L:	ratio between the flows of streams Light and Feed.
γ:	generic operational constraints.
ΔT:	temperature difference between steam and liquid.
ΔP:	pressure drop trough the filter.
Δt:	total processing and maintenance time.
δx:	maximum allowed change in decision variables at each RTE execution.
δt:	time between RTE execution.
δt_a:	value from which further improvement by decreasing δt values is not perceptible.
ε:	void fraction.
θ:	integration auxiliar variable.
θ_d:	pure delay constant.
Φ:	generic objective function dependant of the system trajectory.
φ:	generic dynamic process model.
κ:	quality parameter.
λ:	latent heat of steam.
μ:	fluid viscosity.
ξ:	relative error in the nominal parameter value (to emulate plant-model mismatch).
ρ:	fluid density.
σ:	standard deviation for nominal parameter value (to emulate variability).
τ_l:	first order time constant.
τ_m:	time devoted to maintenance.
υ_s:	superficial flow rate for the liquid flowing trough the filtration cake.
ω:	feed concentration, expressed as the mass of solid per unit of volume filtered.

Bibliography

J. Albuquerque and L. Biegler. Data reconciliation and gross error detection for dynamic system. *AIChE J.*, 42(10):2841, 1995.

S. Alekman. How can steady-state be identified automatically? *Cont. Proc. Industries*, 8:2, 1994.

A. Alle and J. Pinto. Mixed-integer programming models for the scheduling and operational optimization of multiproduct continuous plants. In *DYCOPS*, page 213, 2001.

A. Alle, J. Pinto, and L. Papageourgiou. *Computer Aided Chemical Engineering*, volume 10. Elsevier, Amsterdam, 2002.

G. Almasy and T. Sztano. Checking and correction of measurements on the basis of linear system models. *Probl. Control Inf. Theory*, 4(1):57, 1975.

AspenTech. *Aspen Custom Modeler v10.1 Reference Manual*. Aspen Technology, Inc., Cambridge, MA., 1998.

J. Ayala. State of the art in CLRTO. In *AspenWorld 97 Conf. Proc.*, Boston, MA, 1997.

R. Backer, S. Hall, and B. Rustem. Robust optimal decisions with stochastic non-linear economic systems. *J. Economics Dynamics and Control*, 18:125, 1994.

M. Bagajewicz. A brief review of recent developments in data reconciliation and gross error detection/estimation. *Latin Am. App. Res.*, 30:335, 2000.

M. Bagajewicz and Q. Jiang. Integral approach to plant linear dynamic reconciliation. *AIChE J.*, 43:2546, 1997.

J. Balchen. How have we arrived at the present state of knowledge in process control? Is there a lesson to be learned? *J. of Proc. Control*, 9:101, 1999.

P. Barton. *The modelling and simulation of combined discrete/continuous processes*. PhD thesis, University of London, London SW7 2BY, 1992.

P. Barton and C. Pantelides. Modelling of combined discrete/continuous processes. *AIChE J.*, 40(6), 1994.

K. Basak, K. Abhilash, S. Ganguly, and D. Saraf. On-line optimization of a crude distillation unit with constraints on product properties. *Ind. Eng. Chem. Res.*, 41:1557, 2002.

M. Bayles. Rigorous crude unit optimization. In *Aspen World Users Group Meeting*, Houston, TX, 1996. AspenTech AC&O Division.

V. Becerra, P. Roberts, and G. Griffiths. Novel developments in process optimization using predictive control. *J. Proc. Control*, 8(2):117, 1998.

J. Bernard. Plant control at the right level. *Control Eng.*, Sept., 1966.

J. Bernard and G. Howard. Organizing multilevel process control systems. *Automation*, March, 1970.

H. Besl, W. Kossman, T. Crowe, and M. Caracotsios. Nontraditional optimization for isom unit improves profits. *Oil & Gas J.*, 96(19):61, 1998.

L. Biegler. Strategies for simultaneous solution and optimization of differential-algebraic systems. In J. Siirola, I. Grossman, and G. Stephanopoulos, editors, *FOCAPD*, page 155. CACHE-Elsevier, 1990.

L. Biegler. Tailoring optimization algorithms to process applications. *Comp. Chem. Eng.*, 16 Suppl.:S81, 1992.

L. Biegler, I. Grossmann, and A. Westerberg. A note on approximation techniques used for process optimization. *Comp. Chem. Eng.*, 9:201, 1985.

D. Borio, M. Menendez, and J. Santamaria. Simulation and optimization of a fixed bed reactor operating in cocking-regeneration cycles. *Ind. Eng. Chem. Res.*, 31:2699, 1992.

D. Borio and N. Schbib. Simulation and optimization of a set of catalytic reactors used for dehydrogenation of butene into butadiene. *Comp. Chem. Eng.*, 19 Suppl.:S345, 1995.

G. Box and N. Draper. *Evolutionary Operation: A Statistical Method for Process Improvement*. Wiley, New York, 1969.

B. Braunschweig, C. Pantelides, H. Britt, and S. Sama. Open software architectures for process modeling: Current status and future perspectives. In *FOCAPD'99*, Colorado, USA, 1999.

H. Britt and R. Luecke. The estimation of parameters in nonlinear, implicit models. *Technometrics*, 15(2):233, 1973.

A. Brooke, D. Kendrick, and A. Meeraus. *GAMS - A Users' Guide*. The Scientific Press, Redwood City, C. A., 1998.

P. Brown and R. Rhinerhart. Automated steady-state identification in multivariable systems. *Hydrocarbon Process.*, Sept.:79, 2000.

C. Broyden. The convergence of a class of double-rank minimization algorithms. *J. Inst. Math. Appl.*, 6:76, 1970.

G. Buzzi, M. Morbidelli, P. Forzatti, and Carra. S. Deactivation of catalysts III: Mathematical models for the control and optimization of reactors. *Int. Chem. Eng.*, 24(3):441, 1984.

S. Cao and R. Rhinehart. An efficient method for on-line identification of steady-state. *J. Proc. Control*, 5:363, 1995.

S. Cao and R. Rhinehart. Critical values for a steady-state identifier. *J. Proc. Control*, 7:149, 1997.

E. Casado. Model optimizes exchanger cleaning. *Hydrocarbon Process.*, 79 (Aug):71, 1990.

M. Castilla, A. Gayubo, A. Aguayo, J. Arandes, and J. Bilbao. Simulation and optimization of methanol transformation into hydrocarbons in a isothermal fixed-bed reactor under reaction-regeneration cycles. *Ind. Eng. Chem. Res.*, 31:2699, 1992.

X. Chen. *The optimal implementation of on-line optimisation for chemical and refinery processes*. PhD thesis, Lousiana State University, Lousiana, 1998.

X. Chen, R. Pike, T. Hertwig, and J. Hopper. Optimal implementation of on-line optimization. *Comp. Chem. Eng.*, 22 Suppl.:S435, 1998.

J. Cheng and E. Zafiriou. Robust model-based iterative feedback optimization of steady state plant operations. *Ind. Eng. Chem. Res.*, 39:4215, 2000.

M. Chiari, G. Bussani, M. Grottoli, and S. Pierucci. On-line data reconciliation and optimisation: refinery applications. *Comp. Chem. Eng.*, 21 Suppl.:S1185, 1997.

A. Contino. Improve plant performance via statistical process control. *Chem. Eng.*, July, 1987.

G. Coombes, K. Randall, and J. Wiseman. Pulp mill set point control system. In *ACC conference*, 1983.

E. Crow, F. Davis, and M. Maxwell. *Statistics Manual*. Dover Publicactions, New York, 1955.

C. Crowe. Reconciliation of process rates by matrix projection Part II: The non-linear case. *AIChE J.*, 32(4):616, 1986.

C. Crowe. Observability and redundancy of process data for steady state reconciliation. *Chem. Eng. Sci.*, 44:2909, 1989.

C. Crowe. Data reconciliation - progresses and challenges. *J. Proc. Control*, 6:89, 1996.

C. Crowe, Y. García Campos, and A. Hrymak. Reconciliation of process flow rates by matrix projection Part I: Linear case. *AIChE J.*, 29:881, 1983.

R. Crowther, J. Pitrak, and E. Ply. Computer control at American Oil II: Application to the process unit. *Chem. Eng. Prog.*, 57(6):39, 1961.

J. Cuthrell and L. Biegler. Simultaneous optimization and solution methods for batch reactor control profiles. *Comp. Chem. Eng.*, 13 Suppl.(1/2):S49, 1989.

C. Cutler and R. Perry. Real-time optimization with multi variable control is required to maximize profits. *Comp. Chem. Eng.*, 7:663, 1983.

M. Darby and D. White. On-line optimization of complex processes. *Chem. Eng. Prog.*, 84(10): 51, 1988.

S. De Hennin, J. Perkins, and G. Barton. Structural decisions in on-line optimization. In *PSE-94*, page 297, Kyougju, Korea, 1994.

I. Dedopoulos and N. Shah. Optimal short-term scheduling of maintenance and production for multipurpose plants. *Ind. Eng. Chem. Res.*, 34:192, 1995.

J. Dimitratos, C. Georgakis, M. El-Aasser, and A. Klein. Dynamic modeling and state estimation for an emulsion co-polymerization reactor. *Comp. Chem. Eng.*, 13 Suppl.(1/2):S21, 1989.

V. Dimitriadis, N. Saha, and C. Pantelides. Modelling and safety verification of discrete/continuous processing systems. *AIChE J.*, 43(4):1041, 1997.

A. Drud. CONOPT- A large-scale GRG code. *ORSA J. on Computing*, 6:207, 1992.

D. Eckman and I. Lefkowitz. A report on optimizing control of a chemical process. *Cont. Eng.*, 3 (Nov):83, 1956.

T. Edgar, D. Himmelblau, and L. Lasdon. *Optimization of chemical processes*. McGraw-Hill, second edition, 2001.

N. Epstein. Optimum evaporator cycle with scale formation. *Can. J. Chem. Eng.*, 57:659, 1979.

C. Filippi-Bossy, J. Bordet, J. Villermaux, S. Marchal-Brassely, and C. Georgakis. Batch reactor optimization by use of tendency models. *Comp. Chem. Eng.*, 13 Suppl.(1/2):S35, 1989.

R. Fletcher. A new approach to variable metric algorithms. *Comput. J.*, 13:317, 1970.

F. Forbes and T. Marlin. Design cost: A systematic approach to technology selection for model-based real -time optimization systems. *Comp. Chem. Eng.*, 20(6/7):717, 1994a.

F. Forbes and T. Marlin. Design criteria for model-based real-time optimization systems. In *PSE-94*, page 133, Kyougju, Korea, 1994b.

F. Forbes, T. Marlin, and J. MacGregor. Model selection criteria for economics-based optimizing control. *Comp. Chem. Eng.*, 18:497, 1994.

Y. Friedman. What's wrong with unit closed loop optimization? *Hydrocarbon Process.*, October: 107, 1995.

D. Fylstra, L. Lasdon, J. Watson, and A. Waren. Design and use of the Microsoft Excel solver. *Interfaces*, 28(5):29, 1998.

D. Geddes and T. Kubera. Integration of planning and real time optimization in olefins production. *Comp. Chem. Eng.*, 24:1645, 2000.

M. Georgiadis and L. Papageorgiou. *Computer Aided Chemical Engineering*, volume 8, page 1111. Elsevier, 2000a.

M. Georgiadis and L. Papageorgiou. Optimal energy and cleaning management in heat exchanger networks under fouling. *Chem. Eng. Res. Des.*, 79:168, 2000b.

M. Georgiadis, L. Papageorgiou, and S. Machietto. Optimal cyclic cleaning scheduling in heat exchanger networks under fouling. *Comp. Chem. Eng.*, 23 Suppl.:S203, 1999.

A. Georgiou, F. Krambeck, T. Cheng, and C. Hene. Closed-loop real-time optimization (CLRTO) reaps economic and operations benefits for FCC-Alky complex. In *NPRA Computer Conference*, Kansas City, KS, 1999.

A. Georgiou, A. Sapre, P. Taylor, R. Galloway, and L. Casey. Ethylene optimization system reaps operations and maintenance benefits. *Oil & Gas J.*, 96(10):46, 1998.

E. Gijsbrechts. Hierarchical approach to organizational problems. *Large Scale Systems*, 8:87, 1985.

D. Goldfarb. A family of variable metric methods derived by variational means. *Math. Comput.*, 24:23, 1970.

M. Guay, S. Kansal, and J. Forbes. Trajectory optimization for flat dynamic systems. *Ind. Eng. Chem. Res.*, 40:2089, 2001.

Y. Haimes and D. Wismer. A computational approach to the combined problem of optimization and parameter estimation. *Automatica*, 8:337, 1972.

M. Hardin, A. Joshi, and J. Jones. Rigorous crude unit optimization. In *NPRA Computer Conference*, 1995.

M. Harold and B. Ogunnaike. Process engineering in the evolving chemical industry. *AIChE J.*, 46(11):2123, 2000.

P. Honig. *Principles of Sugar Technology*, volume III. Elsevier, Amsterdam, 1969.

K. Hou, Y. Li, J. Shen, and S. Hu. Delayed sampling approach to stochastic programming in chemical processes. In *PSE'2000 Conferece*, 2000.

K. Hou, Y. Li, J. Shen, and S. Hu. Crude distillation unit online optimization. *Hydrocarbon Process.*, June:69, 2001.

T. Ishikawa, Y. Natori, L. Uberis, and C. Pantelides. Modelling and optimization of an industrial batch process for the production of dioctyl phthalate. *Comp. Chem. Eng.*, 21 Suppl.:S1239, 1997.

V. Jain and I. Grossmann. Cyclic scheduling of continuous parallel process units with decaying performance. *AIChE J.*, 44:1623, 1998.

S. Jang, B. Joseph, and H. Mukai. On line optimization of constrained multivariable process. *AIChE J.*, 33(1):26, 1987.

A. Jazwinski. *Stochastic Processes and Filtering Theory*. Academic Press, New York, 1970.

G. Jubien and G. Bihary. How can steady-state be identified automatically? *Control Proc. Industries*, 8:64, 1994.

J. Kadam, M. Schlegel, W. Marquardt, R. Tousain, D. van Hessem, J. van den Berg, and O. Bosgra. *Computer Aided Chemical Engineering*, volume 10, page 511. Elsevier, Amsterdam, 2002.

I. Kim, T. Edgar, and N. Bell. Parameter estimation for a laboratory water-gas-shift reactor using a nonlinear error-in-variables method. *Comp. Chem. Eng.*, 15(5):361, 1991.

I. Kim, M. Liebman, and T. Edgar. Robust error-in-variables estimation using nonlinear programming techniques. *AIChE J.*, 36(7):985, 1990.

J. Koninckx. *On-line optimization of chemical plants using steady state models*. PhD thesis, University of Maryland, College Park, 1988.

A. Kretsovalis and R. Mah. Observability and redundancy classification in generalized process networks I: Theorems. *Comp. Chem. Eng.*, 12:671, 1988a.

A. Kretsovalis and R. Mah. Observability and redundancy classification in generalized process networks II: Algorithms. *Comp. Chem. Eng.*, 12:689, 1988b.

S. Krishnan, G. Barton, and J. Perkins. Robust parameter estimation in on-line optimization - Part I: Methodology and simulation case study. *Comp. Chem. Eng.*, 16:545, 1992.

M. Krothapally and S. Palanki. A neural network strategy for batch process optimization. *Comp. Chem. Eng.*, 21 Suppl.:S463, 1997.

D. Kuehn and H. Davidson. Computer control at american Oil I: Mathematics of control. *Chem. Eng. Prog.*, 57(6):44, 1961.

T. Larsson, K. Hestetun, E. Hovland, and S. Skogestad. Self-optimizing control of large-scale plant: The Tennessee Eastman process. *Ind. Eng. Chem. Res.*, 40:4889, 2001.

L. Lasdon and T. Baker. The integration of planning, scheduling and process control. In M. Morari and T. McAvoy, editors, *3th ICCPC*, Asilona, CA, 1986.

P. Latour. *AIChE Symp. Ser.*, volume 94, page 297. 1998. FOCAPO.

V. Lauks, R. Vasbinder, P. Vallenburg, and C. van Leuwen. On-line optimization of an ethylene plant. *Comp. Chem. Eng.*, 16 Suppl.:S213, 1992.

M. Lee, Ch. Han, and K. Chang. Hierarchical time-optimal control of a continuous copolymerization reactor during start-up or grade change operation using genetic algorithms. *Comp. Chem. Eng.*, 21 Suppl.:S1037, 1997.

W. Lee, J. Christensen, and D. Rudd. Design variable selection to simplify process calculations. *AIChE J.*, 12(6):1104, 1966.

M. Liebman, T. Edgar, and L. Lasdon. Efficient data reconciliation and estimation for dynamic processes using nonlinear programming techniques. *Comp. Chem. Eng.*, 16(10/11):963, 1992.

J. Loar. How can steady-state conditions be identified automatically? *Control Proc. Industries*, 8:62, 1994.

C. Loeblein and J. Perkins. Economic analysis of different structures of on-line process optimization systems. *Comp. Chem. Eng.*, 20 Suppl.:S551, 1996.

C. Loeblein and J. Perkins. Economic analysis of different structures of on-line process optimization systems. *Comp. Chem. Eng.*, 22:1257, 1998.

R. MacDonal and C. Howat. Data reconciliation and parameter estimation in plant performance analysis. *AIChE J.*, 34(1):1, 1988.

F. Madron. *Process plant performance. Measurement and Data Processing for Optimization and Retrofits*. Hellis Horwood, 1992.

R. Mah. *Chemical Process Structures and Information Flows*. Butterworth Publishers, Stoneham, MA, 1990.

R. Mah, G. Stanley, and D. Downing. Reconciliation and rectification of process flow and inventory data. *Ind. Eng. Chem. Proc. Des. Dev.*, 11:175, 1976.

R. Mah and A. Tamhane. Detection of gross errors in process data. *AIChE J.*, 28:828, 1982.

T. Marlin. *Process control: designing processes and control systems for dynamic performance*. McGraw-Hill, 1995.

I. Miletic and T. Marlin. Results analysis for real-time optimization: deciding when to change the plant operation. *Comp. Chem. Eng.*, 20 Suppl.:S1071, 1996.

I. Miletic and T. Marlin. On-line stadistical results analysis in Real-time operations optimization. *Ind. Eng. Chem. Res.*, 37(9):3670, 1998.

A. Mizoguchi, T. Marlin, and A Hrymak. Operations optimization and control design for a petroleum distillation process. *Can. J. Chem. Eng.*, 73:896, 1995.

H. Muller-Steinhagen. Mitigation of process heat exchanger fouling. *Chem. Eng. Res. Des.*, 76: 97, 1998.

K. Muske and T. Edgar. *Non linear process control*. Prentice-Hall, Englewood Cliffs, NJ, 1998.

S. Narasimhan, C. Kao, and R. Mah. Detecting changes in steady states using the mathematical theory of evidence. *AIChE J.*, 33:1930, 1987.

S. Narasimhan and R. Mah. Generalized likelihood ratio method for gross error identification. *AIChE J.*, 33(9):1514, 1987.

S. Narasimhan, R. Mah, A. Tamhane, J. Woodward, and J. Hale. A composite statistical test for detecting changes of steady state. *AIChE J.*, 32(9):1409, 1986.

L. Narraway, J. Perkins, and G. Barton. Interaction between process design and process control: economic analysis of process dynamics. *J. Proc. Control*, 1:243, 1991.

R. Nath and Z. Alzein. On-line dynamic optimization of olefins plants. *Comp. Chem. Eng.*, 24: 533, 2000.

S. Nogita. Statistical tests and adjustment of process data. *Ind. Eng. Chem. Process Des. Dev.*, 2:197, 1972.

J. Ocon and G. Tojo. *Problemas de Ingeniería Química*, volume II. Aguilar, 1977. In Spanish.

B. O'Donnell, B. Barna, and C. Gosling. Optimize heat exchanger cleaning schedules. *Chem. Eng. Prog.*, 97(6):56, 2001.

C. Pedersen, D. Mudt, J. Bailey, and J. Ayala. Closed-loop real-time optimization of a hydrocracker complex. In *NPRA Computer Conference*, Nashville, TN, 1995.

A. Pendleton. Computer control at American Oil III: The computer system. *Chem. Eng. Prog.*, 57(6):48, 1961.

J. Perkins. *AIChE Symp. Ser.*, volume 94 of *320*, chapter Plant-wide optimization: opportunities and challenges, page 15. 1998.

L. Pibouleau, P. Floquet, S. Domenech, and C. Azzaro-Pantel. A survey of optimization tools through ESCAPE symposia. *Comp. Chem. Eng.*, Suppl.:S495, 1999.

J. Pinto and I. Grossmann. Optimal cyclic scheduling of multistage multiproduct plants. *Comp. Chem. Eng.*, 18:797, 1994.

E. Pistikopoulos, C. Vassiliadis, J. Arvela, and L. Papageorgiou. Interactions of maintenance and production planning for multipurpose process plants-A system effectiveness approach. *Ind. Eng. Chem. Res.*, 40:3195, 2001.

L. Puigjaner. An integrated framework for real time simulation and optimization of batch processes. *Trends Chem. Eng.*, 7, 2001.

S. Qin and T. Badgwell. *AIChE Symp. Ser.*, volume 93 of *316*, page 232. 1997.

S. Qin and T. Badgwell. An overview of non-linear model predictive control applications. In *Workshop on NMPC*, Ascona, Switzerland, 1998.

C. Rao and J. Rawlings. Steady states and constraints in model predictive control. *AIChE J.*, 45 (6):1266, 1999.

T. Reg Bott. To foul or not to foul, that is the question. *Chem. Eng. Prog.*, November:30, 2001.

P. Reilly and R. Carpani. Application of statistical theory of adjustement to material balances. In *13th Can. Chem. Eng. Conf.*, Montreal, 1963.

G. Reklaitis. Computer-Aided design and operation of batch processes. *Chem. Eng. Educ.*, 29: 76, 1995.

J. Riggs and M. Hetzel. Real time refinery-wide optimization. In *AIChE Annual Meeting*, Los Angeles, CA, 2000.

D. Ripps. *Chem. Eng. Prog. Symp. Ser.*, volume 61. AIChE, 1965.

P. Roberts. An algorithm for steady-state system optimization and parameter estimation. *Int. J. Sys. Sci.*, 10(7):719, 1979.

P. Roberts and T. Williams. On an algorithm for combined system optimization and parameter estimation. *Automatica*, 18:199, 1981.

D. Robertson, J. Lee, and J. Rawlings. A moving horizon-based approach for least squares state estimation. *AIChE J.*, 4(8):2209, 1996.

D. Rollins and J. Davis. Unbiased estimation of gross errors in process measurements. *AIChE J.*, 38(4):563, 1992.

D. Rollins and J. Davis. Gross error detection when variance-covariance matrices are unknown. *AIChE J.*, 39(8):1335, 1993.

J. Romagnoli and M. Sanchez. *Data processing and reconciliation for chemical processes operation*. Academic Press, New York, 1999.

J. Romero, A. Espuña, F. Friedler, and L. Puigjaner. A new framework for batch process optimization using the flexible recipe". *Ind. Eng. Chem. Res.*, 42(2):370, 2003.

E. Rosen and L. Partin. A perspective: The use of the spreadsheet for chemical engineering computations. *Ind. Eng. Chem. Res.*, 39:1612, 2000.

D. Rudd and C. Watson. *Strategy of Process Engineering*. John Wiley & Sons, 1968.

M. Sánchez and M. Bagajewicz. On the impact of corrective maintenance in the design of sensor networks. *Ind. Eng. Chem. Res.*, 39(4):977, 2000.

E. Sanmartí, A. Espuña, and L. Puigjaner. Batch production and preventive scheduting under equipment failure uncertainty. *Comp. Chem. Eng.*, 21:1157, 1997.

E. Schulz, S. Diaz, and A. Bandoni. *Computer Aided Chemical Engineering*, volume 8, page 487. Elsevier, Amsterdam, 2000.

W. Seider, J. Seader, and D. Lewing. *Process Design Principles: Synthesis, Analysis, and Evaluation*. John Wiley & Sons, 1999.

D. Shanno. Conditioning of quasi-newton methods for function minimization. *Math. Comput.*, 24:647, 1970.

A. Sheikh, S. Zubari, M. Haq, and M. Budair. Reliability-based maintenance strategies for heat-exchangers subject to fouling. *Trans. ASME*, 118:306, 1996.

R. Sivasubramanian and W. Penrod. Computer control for third world countries: fantasy or reality? *Hydrocarbon Process.*, August:84c, 1990.

S. Skogestad and I. Halvorsen. Self-optimizing control: basis issues and Taylor series analysis. In *COSY Workshop*, Makedonia, 1998.

F. Smaïli, D. Angadi, C. Hatch, O. Herbert, V. Vassiliadis, and D. Wilson. Optimization of scheduling of cleaning in heat exchanger networks subject to fouling: sugar industry case study. *Chem. Eng. Res. Des.*, 77(2):159, 1999.

F. Smaïli, V. Vassiliadis, and D. Wilson. Mitigation of fouling in refinery heat exchanger networks by optimal management or cleaning. *Energy and Fuels*, 15:1038, 2001.

R. Sorensen and C. Cutler. LP integrates economics into dynamic matrix control. *Hydrocarbon Process.*, September:57, 1998.

G. Stanley and R. Mah. Observability and redundancy in process data estimation. *Chem. Eng. Sci.*, 36:259, 1981.

M. Taskar and J. Riggs. Modeling and optimization of a semiregenerative catalytic naphtha reformer. *AIChE J.*, 43(3):740, 1997.

ISA. The Instrumentation System and Automation Society. *ISAdS88.01 Part 1: Models and Terminology*. International Soc. for Measurement and Control, 1995.

ISA. The Instrumentation System and Automation Society. *ISAdS95.01 Part 1: Models and Terminology*. International Soc. for Measurement and Control, 1999.

I. Tjoa and L. Biegler. Reduced successive quadratic programming strategy for errors-in-variables estimation. *Comp. Chem. Eng.*, 16(6):523, 1992.

I. Tjoa, Y. Ota, H. Matsuo, and Y Natori. Ethylene plant scheduling system based on a MINLP formulation. *Comp. Chem. Eng.*, 21 Suppl.:S1073, 1997.

H. Tong and C. Crowe. Detecting persistent gross erros by sequential analysis of principal components. *AIChE J.*, 43(5):1242, 1997.

A. Tresmondi, A. Domingues, and R. Maciel Filho. *Computer Aided Chemical Engineering*, volume 9, page 805. Elsevier, 2001.

M. Tvrzská and D. Odloak. One-layer real time optimization of LPG production in the FCC unit: Procedure, advantages and disadvantages. *Comp. Chem. Eng.*, 22 Suppl.:S191, 1998.

V. Václavek. Studies on system engineering III: Optimal choice of the balance measurements in complicated chemical systems. *Chem. Eng. Sci.*, 24:947, 1969.

R. Van Wijk and M. Pope. Advanced process control and on-line optimization in Shell refineries. *Comp. Chem. Eng.*, 16 Suppl.:S69, 1992.

C. Vassiliadis and E. Pistikopoulos. Maintenance scheduling and process optimization under uncertainty. *Comp. Chem. Eng.*, 25:217, 2001.

D. White. On line optimization: what, where and estimating ROI. *Hydrocarbon Process.*, June: 43, 1997.

D. White. On line optimization: what have we learned? *Hydrocarbon Process.*, June:55, 1998.

T. Williams and R. Otto. A generalized chemical processing model for the investigation of computer control. *AIEE Trans.*, 79:458, 1960.

A. Willsky and H. Jones. A generalized likelihood ratio approach to the detection and estimation of jumps in linear systems. *IEEE Trans. Autom. Control.*, 21(1):108, 1976.

K. Yamamura, M. Nakajima, and H. Matsuyama. Detection of gross errors in process data using mass and energy balances. *Int. Chem. Eng.*, 28(1):91, 1988.

C. Ying and B. Joseph. Performance and stability analysis of LP-MPC and QP-MPC cascade control systems. *AIChE J.*, 45(7):1521, 1999.

W. Yip and T. Marlin. Designing plant experiments for real-time optimization system. In *AIChE Annual Meeting*, Los Angeles, CA, 2000. AIChE.

W. Yip and T. Marlin. Multiple data sets for model updating in real-time operations optimization. *Comp. Chem. Eng.*, 26:1345, 2002.

S. Yoon, S. Dasgupta, and G. Mijares. Real-Time optimization boosts capacity of Korean olefins plant. *Oil & Gas J.*, 94:36, 1996.

A. Zanin, M. Tvrzská de Gouvêa, and D. Odloak. Inustrial implementation of a real-time optimisation strategy for maximizing production of LPG in a FCC unit. *Comp. Chem. Eng.*, 24: 525, 2000.

Y. Zhang and F. Forbes. Extended design cost: performance criterion for real-time optimization system. *Comp. Chem. Eng.*, 24:1829, 2000.

Y. Zhang, D. Nadler, and F. Forbes. Results analysis for trust constrained real-time optimization. *J. Proc. Control*, 11(3):329, 2001.

Y. Zhang, D. Nadler, and F. Forbes. Real-time optimization under parametric uncertainty: a probability constrained approach. *J. Proc. Control*, 12:373, 2002.

S. Zubari, A. Sheikh, M. Budair, and M. Badar. A maintenance strategy for heat transfer equipment subject to fouling: A probabilistic approach. *J. Heat Transfer*, 119:575, 1997.

Appendix A

Managing the Uncertainty

Introduction

As commented in section 1.4.2 (page 12), on-line optimisation systems have poor long-term service factor due, at least partially, to inadequate optimisation robustness. Although most RTO systems attempt to improve model accuracy through model updating, this is, update some of the model's parameters, these ones, as any information flowing into the loop, have associated some degree of uncertainty. In section section 2.6 (page 34) it has been mentioned that the uncertainty in on-line optimisation systems is associated mainly to measurements, model parameters and changes in unmeasured variables that are assumed to a constant value.

A possible way of dealing with that uncertainty is to using a chance constrained approach. Assuming that there is the following optimisation problem to solve (in the reduced space):

$$\max_{x} \quad IOF(x,p) \tag{A.1}$$

subject to:

$$g(x,p) \leq 0 \tag{A.2}$$

where as usual, p represents the uncertain parameters and x includes the independent variables. Equation A.2 represents the inequality constraints. Thus, when information about the probability density function (pdf)[1] for every parameter p is available, the stochastic version of the problem can be stated as:

$$\max_{x} \quad E\left[IOF(x,p)\right] \tag{A.3}$$

subject to:

[1] To be realistic, when a parameter value is uncertain, the chance of having the pdf available is scarce. Nevertheless, the solution obtained by a probabilistic approach is more conservative than the deterministic one, what may be desirable.

$$\prod [g(x,p) \geq 0] \leq \pi \tag{A.4}$$

In other words, $E[IOF]$, the expected value of the objective function is maximised, while the probability of constrains violation (Π) is keep lower than a given threshold value π (e.g. a 95 % of confidence level).

The solution of such problem is usually cumbersome, because a proper approximation of $E[IOF]$ and Π commonly requires a Monte Carlo simulation using an important set of possible scenarios (using the pdf for every p) at every intermediate solution proposed by the optimisation algorithm. The number of scenarios is virtually infinity, but in practice a big number of them will give satisfactory results. Even though, the problem often require a huge number of objective function and constraints evaluations. Nevertheless, such concepts can be for extension applied to RTE, with the great advantage that RTE only explores a few set of solution around the current one, rather than solving the whole optimisation problem, being therefore less computationally expensive than a stochastic RTO approach. Consequently, for every iteration of the "Robust RTE" (RRTE) the problem is:

$$\begin{array}{ll} max & \overline{IOF}(x_k, p) \\ x_k \forall k & \end{array} \tag{A.5}$$

subject to:

$$f_r [g(x_k, p) \geq 0] \leq \pi \tag{A.6}$$

where k is an small integer number. Thus, for every possible solution x_k, several possible scenarios are generated using the pdf of p. Then, the IOF and the associated constraints g are evaluated, obtaining the associated relative frequency distributions for IOF and g. Therefore, it is possible to evaluate the average value for IOF, $\overline{IOF}$, and the relative frequency of the constraint g violation, f_r. It can be seen that the improvement algorithm is analogous to the introduced in chapter 3. The difference is that for the Robust RTE case, every alternative solution point x_k has associated a number of scenarios rather than a single occurrence (see scheme in figure A.1).

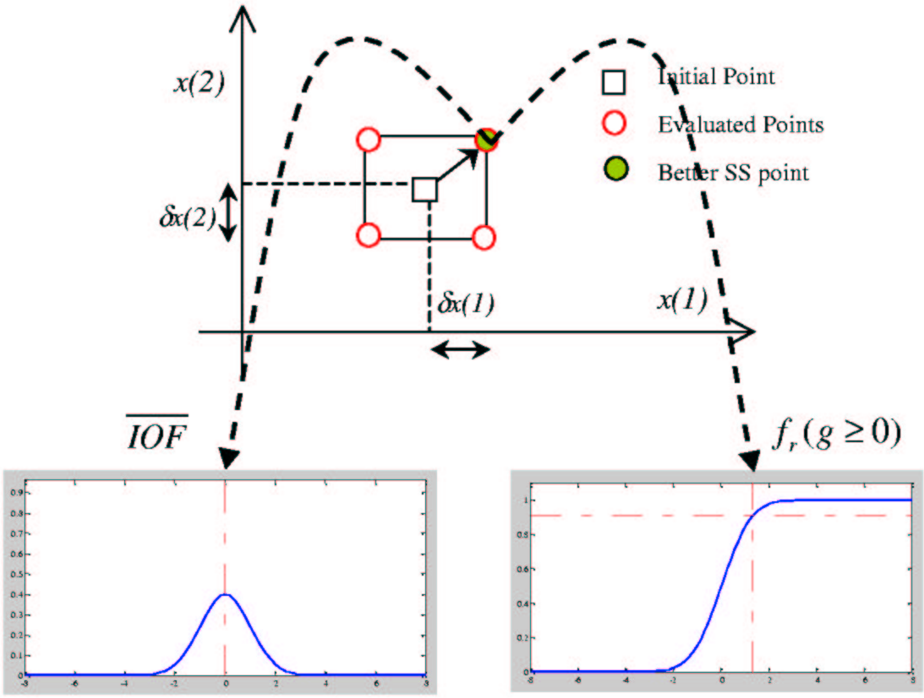

Figure A.1: Robust RTE

Appendix B

Models Used for the Williams-Otto Reactor

Kinetics

Let be:

$$R_1 = V_r \cdot k_1(T_r) \cdot X_a \cdot X_b \tag{B.1}$$

$$R_2 = V_r \cdot k_2(T_r) \cdot X_c \cdot X_b \tag{B.2}$$

$$R_3 = V_r \cdot k_3(T_r) \cdot X_p \cdot X_c \tag{B.3}$$

Mass balances

For the steady state:

Global:

$$F_a + F_b = F_r \tag{B.4}$$

For A:

$$F_a - F_r X_a - R_1 = 0 \tag{B.5}$$

For B:

$$F_b - F_r X_b - R_1 - R_2 = 0 \tag{B.6}$$

For C:

$$-F_r X_c - 2R_1 - R_2 - R_3 = 0 \tag{B.7}$$

For E:

$$-F_r X_e - 2R_2 = 0 \tag{B.8}$$

For P:

$$-F_r X_p + R_2 - \frac{1}{2} R_3 = 0 \tag{B.9}$$

For G:

$$-F_r X_g - \frac{3}{2} R_3 = 0 \tag{B.10}$$

During the transitions:

Global:

$$F_a + F_b - F_r = \frac{d(V_r \cdot \rho)}{dt} = 0 \tag{B.11}$$

For A:

$$F_a - F_r \cdot X_a - R_1 = V_r \cdot \rho \frac{dX_a}{dt} \tag{B.12}$$

For B:

$$F_b - F_r \cdot X_b - R_1 - R_2 = V_r \cdot \rho \frac{dX_b}{dt} \tag{B.13}$$

For C:

$$-F_r \cdot X_c - 2R_1 - R_2 - R_3 = V_r \cdot \rho \frac{dX_c}{dt} \tag{B.14}$$

For E:

$$-F_r \cdot X_e - 2R_1 = V_r \cdot \rho \frac{dX_e}{dt} \tag{B.15}$$

For P:

$$-F_r \cdot X_p + R_2 - \frac{1}{2} R_3 = V_r \cdot \rho \frac{dX_p}{dt} \tag{B.16}$$

For G:

$$-F_r X_g - \frac{3}{2} R_3 = V_r \cdot \rho \frac{dX_g}{dt} \tag{B.17}$$

where:

k_i: kinetic coefficient for reaction i (1/s), whose numerical values are given in section 3.3.1 (page 57).

T_r: reactor temperature (^{o}C).

F_i: i mass flow (kg/s).

X_i: i mass fraction.

ρ: density of the fluid in the reactor (assumed constant at 1 kg/lt).

V_r: reactor volume (assumed constant at 2105 lt).

Appendix C

A Method for On-line Forecasting of ts_{opt}

Another way to look at the problem

The trivial way of perform a forecast of ts_{opt} would be to track the difference between IOF and MOF, obtaining its trend and then use the trend model to anticipate the time at which such difference becomes equal to cero. The clear disadvantage of this approach relies in the non-linearity of such trend (see figure 4.4 in page 78). However, from the equation 4.18 (78):

$$\overbrace{IOF(ts_{opt}) \cdot (ts_{opt} + \tau_m)}^{A_1} - \overbrace{\int_0^{ts_{opt}} IOF(\theta) d\theta - C_m}^{A_2} = A_1 - A_2 = 0 \tag{C.1}$$

and considering that initially $IOF > MOF$, the RHS (Right Hand Side) of this expression will be positive for values of ts lower than ts_{opt}. Using the available information at the moment k:

$$\{i, IOF(i), MOF(i)\} \quad \forall i = 1 \ldots k \tag{C.2}$$

it is possible to obtain the difference between both terms (DOF):

$$A_1(i) - A_2(i) = DOF(i) \quad \forall i = 1 \ldots k \tag{C.3}$$

The use of the A letter for designing the right hand terms is deliberated, because as it is illustrated in Figures C.1 and C.2 their graphical interpretations are areas.

Then, DOF can be plotted against i. For most of the cases analysed of decreasing functions (exponential, quadratic, etc.) this resulting trend plot does is linear. Hence, by using linear fit it is possible to obtain:

$$DOF(i) \approx m(k) \cdot i + b(k) \tag{C.4}$$

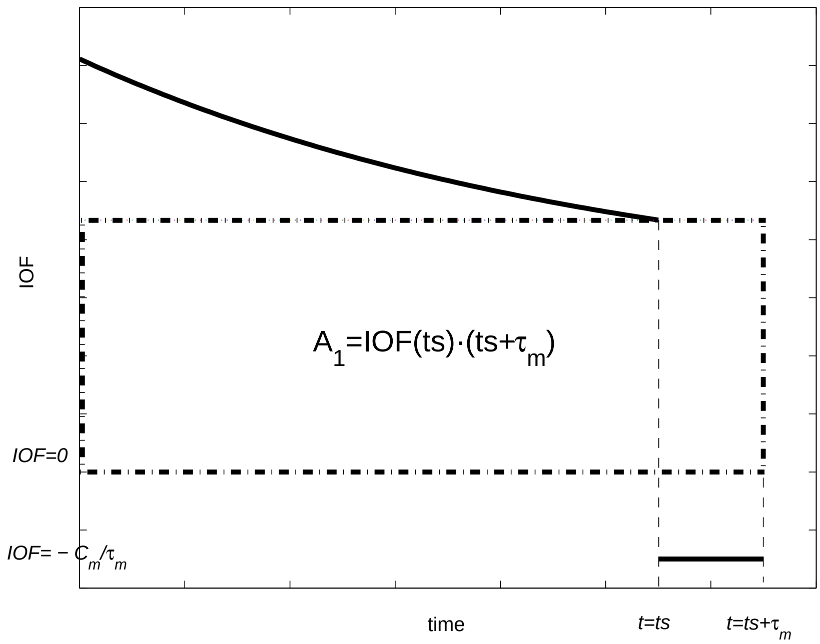

Figure C.1: A_1 is the rectangular area contoured by the dot-dashed lines

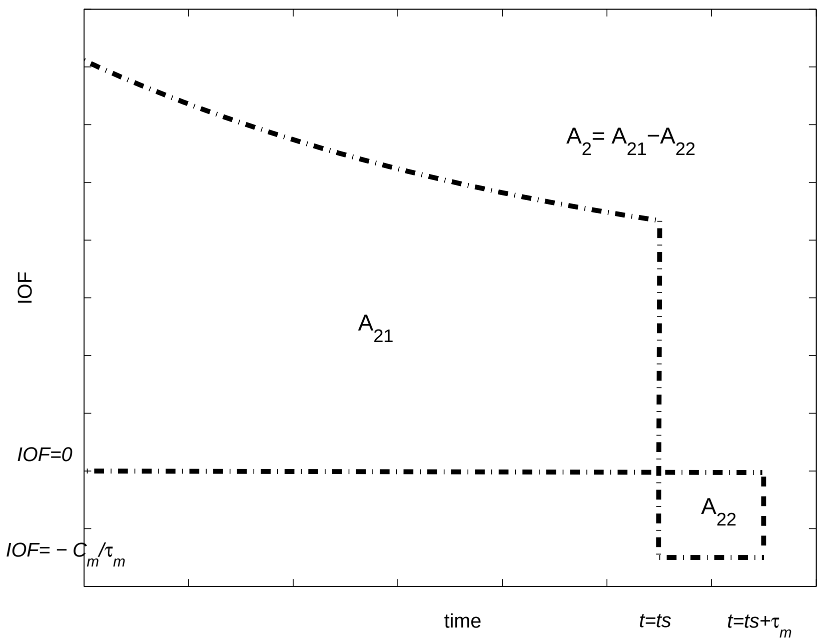

Figure C.2: A_2 is the difference between the two areas contoured by the dot-dashed lines

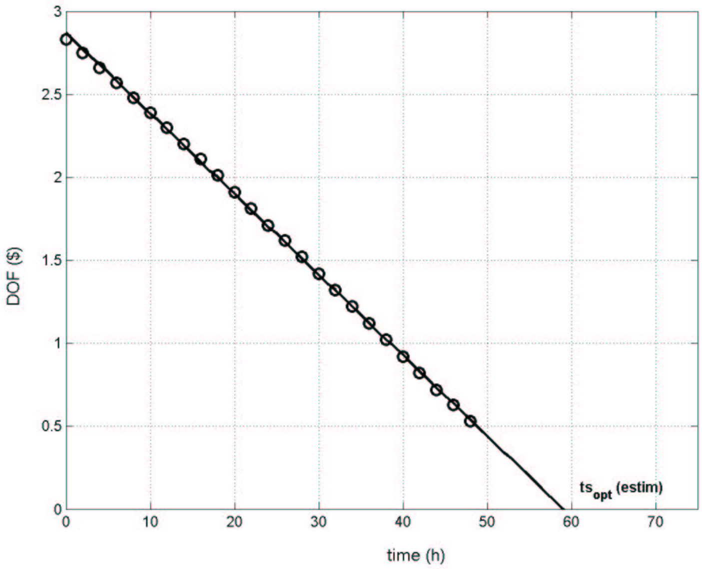

Figure C.3: On-line forecasting of ts_{opt} value

where m and b are functions of k because they can be updated at every k. From that, ts_{opt} means $DOF = 0$ and hence:

$$i_{opt} = \frac{-b(k)}{m(k)} \tag{C.5}$$

where i_{opt} corresponds to the time period associated to ts_{opt}. The basic strategy is shown in the Figure C.3. This estimation becomes more accurate with time, and is very helpful for the resource planning[1].

[1] As a recommendation, when such relation is not linear, both terms ($A_1$and A_2) may be successively multiplied by $(ts+\tau_m)$ until obtaining a linear fit with the desired degree of accuracy. Indeed, DOF can be seen as:

$$DOF(ts) = (ts+\tau_m)^n \cdot [IOF(ts) - MOF(ts)]$$

where n is equal to 1, which is just a way of weighting the differences between IOF and MOF observed in the nearer times (those with higher ts value). The bigger the n value, the bigger the weighting factor, thus the initial high differences are attenuated

Appendix D

Alternative Formulation for the Solution of the Industrial Case Study II

Formulation (for the pre-evaporation section)

According to Jain and Grossmann (1998) a repetitive schedule for cleaning tasks for the pre-evaporation section can be found and the length of this schedule is called as the "cycle time", and is denoted by a continuous variable T_{cycle}. This leads to a cyclic operation, which could be convenient for practical reasons. The resulting MINLP problem, involves the parameters already defined and the following variables:

F_j: Mass flow of juice fed to every evaporator j (*kg/h*).

L_j: Variable used to linearize the mass balances constraints (*kg*).

N_j: Integer variable, denoting the number of sub-cycles for the evaporator j during the time cycle.

T_{cycle}: Cycle time (*h*).

t_j: Total operation time of an evaporator (*h*).

ts_j: Operation time for each sub-cycle (*h*).

$\overline{X}$: Objective function, mean output sugar concentration (*%*)

The objective of this problem is to maximise the mean sugar concentration of the juice leaving the pre-evaporation section that will lead to a higher concentration of the syrup. The following expression can be applied to compute the mean output sugar concentration and then used as the objective function:

$$\overline{X} = \frac{\sum_{j=1}^{p} F_j t_j}{\sum_{j=1}^{p} X_0 + \frac{2a_j T_j A_j \cdot \Delta T_j N_j}{\lambda_j b_j F_j t_j} \left[\left(1 + b_j \frac{t_j}{N_j}\right)^{\frac{1}{2}} - 1 \right]} \tag{D.1}$$

where the operation time for each sub-cycle is given by:

$$ts_j = \frac{t_j}{N_j} \ \ \forall j = 1 \dots p \tag{D.2}$$

Mass balance: The total mass flow of fed juice (F_T) coming from the clarification section must be processed in the evaporators, therefore:

$$F_T T_{cycle} = \sum_{j=1}^{p} F_j t_j \tag{D.3}$$

In order to linearise the above constraint a new variable L_j is used. If F_{lo_j} is the lower and F_{up_j} is the upper bound of feed to be processed then:

$$F_T T_{cycle} = \sum_{j=1}^{p} \left(F_{lo_j} t_j + L_j \right) \tag{D.4}$$

$$L_j \leq \left(F_{up_j} - F_{lo_j} \right) t_j \ \ \forall j = 1 \dots p \tag{D.5}$$

Objective Function: After linearising the mass balance constraint, F_j is substituted in the objective function as follows:

$$\overline{X} = \frac{\sum_{j=1}^{p} \left(F_{lo_j} t_j + L_j \right)}{\sum_{j=1}^{p} X_0 + \frac{2a_j T_j A_j \cdot \Delta T_j N_j}{\lambda_j b_j \left(F_{lo_j} t_j + L_j \right)} \left[\left(1 + b_j \frac{t_j}{N_j}\right)^{\frac{1}{2}} - 1 \right]} \tag{D.6}$$

Processing and Cleaning time: The total time (operating and cleaning time) for evaporator j is given by the following equations:

$$\Delta t_j = N_j \tau_{m_j} + t_j \ \ \forall j = 1 \dots p \tag{D.7}$$

$$\Delta t_j \leq T_{cycle} \ \ \forall j = 1 \dots p \tag{D.8}$$

Bounds:

$$t_{lo} \leq ts_j \leq t_{up} \ \ \forall j = 1 \dots p \tag{D.9}$$

Table D.1: Pre-evaporation section solution using *MP2*

Decision Variables	*A*	*B*	*C*	*D*	*E*
N_j	1	1	1	1	1
$F_j\ (\%/F_T)$	26.53	23.20	23.20	26.53	23.20
$t_j\ (h)$	56.67	58.67	58.67	56.67	58.68
$T_{cycle}\ (h)$	70.67				
Z (%)	26.62				

$$1 \leq N_j \leq N_{up} \ \ \forall j = 1 \dots p \tag{D.10}$$

$$L_j \geq 0 \ \ \forall j = 1 \dots p \tag{D.11}$$

The MINLP problem (*MP2*) comprises then the objective function (equation D.6) and the last five equations as linear constraints (equations D.7 to D.11).

Results

The solution to the problem given in the data of table 5.4 (page 121) is obtained by solving the whole formulation *MP2* using SBB (a NLP based branch and bound algorithm, Brooke et al. (1998)), in the GAMS modelling environment.[1] The best solution found is summarised in the table D.1.

It is worth mentioning that besides that the formulation involves an additional variable (in comparison with the proposed *MP1* in chapter 5) and the presence of some integers, the optimum found is starting point dependent, as is indicated by the histogram of figure D.1.

As already mentioned in chapter 4, the solution found depends directly on the upper bound in T_{cycle} (as well of that of N). Such behaviour can be explained conceptually: the solution given in table D.1 is totally equivalent to the set of solutions that have as decision variables values (T_{cycle}, t_j and N_j) k times the given in such table, being k any positive integer. For intermediate values of T_{cycle}, the solutions are always poorer because another entire cycle does not “fit” in the current time horizon (i.e. figure D.2).

[1] It takes between 1 and 1.5 seconds to solve every problem in a AMD-K7 processor with 128 Mb RAM at 600 MHz, and about 4 seconds in an spreadsheet environment using an implementation of GRG2.

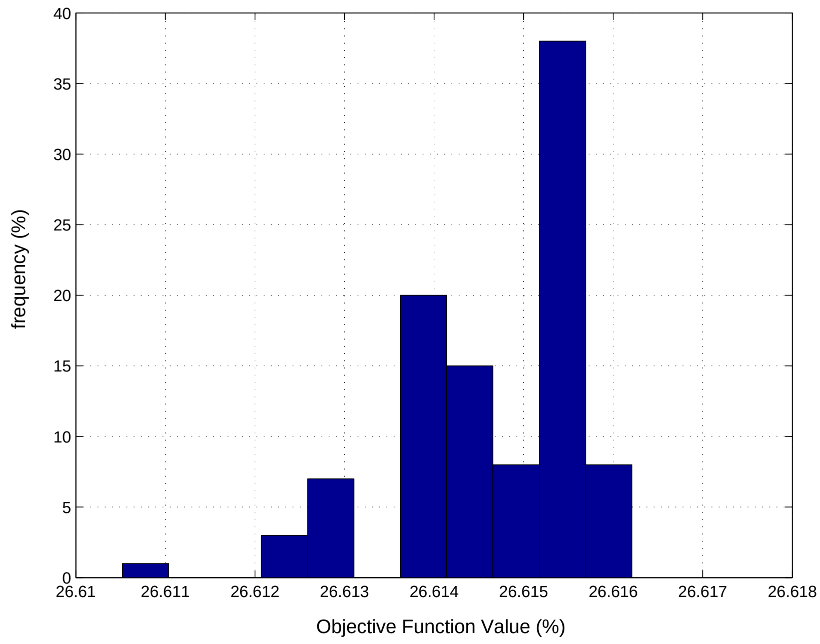

Figure D.1: Results obtained when solving *MP2* from random starting points

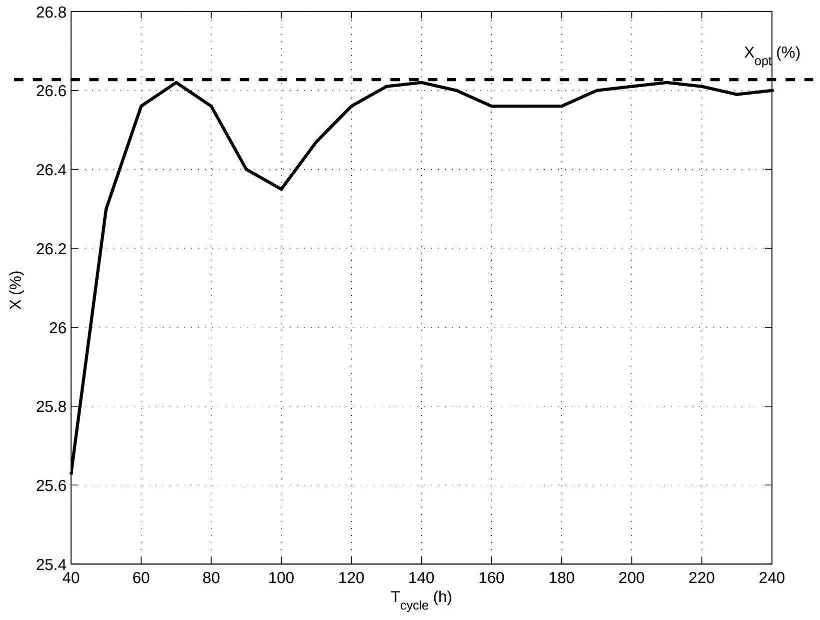

Figure D.2: Output sugar concentration when solving *MP2* using T_{cycle} as a parameter

Appendix E

About the Pseudo Steady State Assumption in the Industrial Case II

Balance dynamics

The dynamic behaviour of an evaporator such as that in section 5.3.2.1 (page 117), may be better described by the following equations corresponding to a well mixed situation:

Solid mass balance:

$$\frac{d(MX)}{dts} = FX_0 - F_P X \tag{E.1}$$

Total mass balance:

$$\frac{dM}{dts} = F - F_P - F_V \tag{E.2}$$

Assuming that that:

- The sensible heat can be neglected and,
- Perfect inventory control (typically there is a level controller)

$$F_V \approx \frac{Q}{\lambda} = \frac{\frac{aAT \cdot \Delta T}{\lambda}}{X\sqrt{1+bts}} = \frac{\beta}{X\sqrt{1+bts}} \tag{E.3}$$

$$\frac{dM}{dts} = 0$$

from where the following differential expression of X can be obtained:

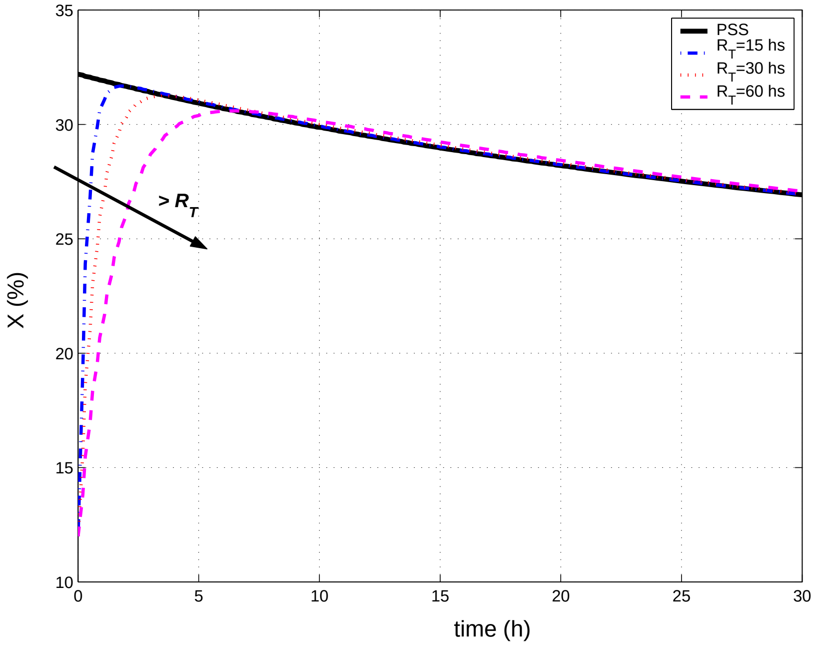

Figure E.1: About the pseudo steady state (PSS) hypothesis

Table E.1: Consequences of PSS assumption on the optimisation results

Model	ts_{opt} (h)	$MOF_{opt}(\%)$	Difference in ts_{opt} $(\%)$
PSS	59.1	12.43	-
Dynamic $R_T = 15\,h$	60.0	12.38	1.51
Dynamic $R_T = 30\,h$	61.5	12.31	3.98
Dynamic $R_T = 60\,h$	64.5	12.17	8.74

$$\frac{dX}{dts} + \frac{F}{M}(X - X_0) = \frac{\beta}{X\sqrt{1 + bts}} \tag{E.4}$$

with the initial condition:

$$X|_{ts=0} = X_0 \tag{E.5}$$

The chart in figure E.1 shows the profiles obtained integrating numerically this equation and the corresponding pseudo steady state behaviour for different values of the evaporator capacity, expressed by its residence time, $R_T = \frac{M}{F}\,h$.

After five hours in all cases, the pseudo steady state assumption acceptably represents the evaporator behavior. However, table E.1 clearly illustrates the error produced in the determination of ts_{opt} using such representation, using the pseudo steady state value as a reference.