Design of reactive distillation systems using evolutionary optimisation algorithms: application to the production of ethyl tert-butyl ether (ETBE)

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Introduction

ETBE is an octane-rating enhancing gasoline additive produced by the reaction of isobutene and ethanol, catalysed by acid ion-exchange resins [1]. ETBE is suitable to be produced by reactive distillation (RD). RD is a process intensification solution that combines reaction and separation in the same equipment. The design of RD column is complex due to its nonlinearity and existence of integer variables. Optimisation-based methods are seen as the most rigorous for RD column design.

Objectives

- To develop and validate a methodology for RD column design based on a hybrid optimisation-based strategy
- To evaluate the application of the PSO algorithm to solve this design problem

Design Algorithms

- Genetic algorithms are search algorithms inspired by the mechanics of natural selection
- Particle swarm optimisation is a more recent class of search algorithms, inspired by the mechanics of collective animal behaviour

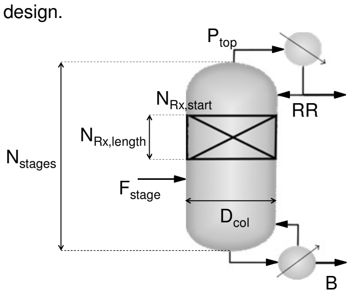


Fig. 1 – RD column design variables.

Problem Formulation

$$\max \mathit{Penalised\,Gross\,Annual\,Profit}\,(GAP) = \mathrm{R_{ETBE}} - (\mathrm{C_{column}} + \mathrm{C_{condenser}} + \mathrm{C_{reboiler}} + \mathrm{C_{steam}} + \mathrm{C_{etoh}} + \mathrm{C_{Raffinate\,1}}) + \mathrm{Penalty}$$

s.t.

RD physical model

ETBE bottom mass fraction ≥ 0.95

$$\mathrm{Penalty\ (M€/year)} = \begin{cases} -15(0.95 - x_{\mathrm{ETBE,bot}})^{0.3}, & x_{\mathrm{ETBE,bot}} < 0.95 \\ 0, & x_{\mathrm{ETBE,bot}} \geq 0.95 \end{cases}$$

Tab. 1 – Evolutionary algorithm parameters used.

Genetic Algorithm		PSO Algorithm	
$N_{individuals}$	30	$N_{particles}$	30
$N_{generations}$	80	$N_{iterations}$	80
$N_{individuals}$ in tournament selection	8	Inertia weight	0.6
α (Blend crossover)	0.3	Best particle weight	1.7
Crossover probability	0.95	Best swarm particle weight	1.7
Mutation probability	0.05		

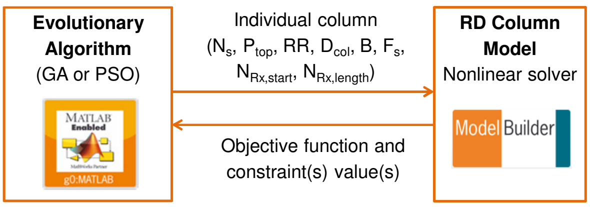


Fig. 2 – Representation of hybrid strategy used for RD column optimisation-based design.

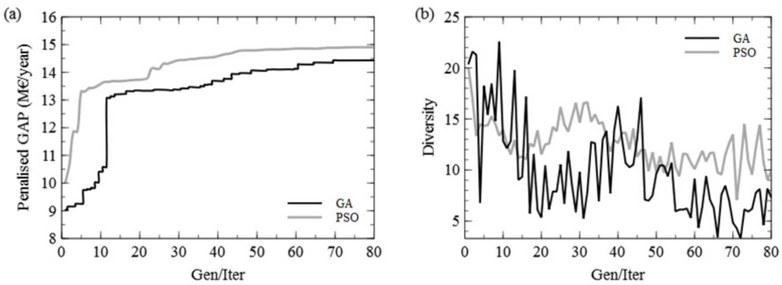
RD Column Model

- MESH equations
- Reactive packing: KATAPK SP-12
- Kinetic model validated in previous work [2]
- Components/lumps considered: Isobutene, ethanol, ETBE, 1-butene, n-butane, water, DIB and TBA

Results

Tab. 2 – RD column configurations, GAP and constraint values obtained.

Design variable	Units	GA column	PSO column
Total number of stages (N_{stages})	-	34	37
Top pressure (P_{top})	bar	9.73	10
Reflux ratio (RR)	-	0.867	1.7
Column diameter (D_{col})	M	1.8	1.8
Bottom molar flowrate (B)	mol/s	15.48	15.65
Feed stage location (F_{stage})	-	25	28
Beginning of reaction zone ($N_{Rx,start}$)	-	5	4
Number of stages of reaction zone ($N_{Rx,length}$)	-	13	24
Gross annual profit (GAP)	M€/year	14.43	14.91
ETBE bottom mass fraction	-	0.952	0.950



$$\mathrm{Diversity} = \sum_{k=1}^{N_{\mathrm{desvar}}} \sum_{m=1}^{N_{\mathrm{ind}}} (z_{k,m} - c_k)^2$$

$$c_k = \sum_{m=1}^{N_{\mathrm{ind}}} z_{k,m}/N_{\mathrm{ind}}$$

$$z_{k,m} = \frac{z'_{k,m} - z'_{k,\min}}{z'_{k,max} - z'_{k,\min}}$$

Fig. 3 – Evolution of the (a) best individual objective function value and (b) population diversity with the number of generations/iterations for both GA and PSO.

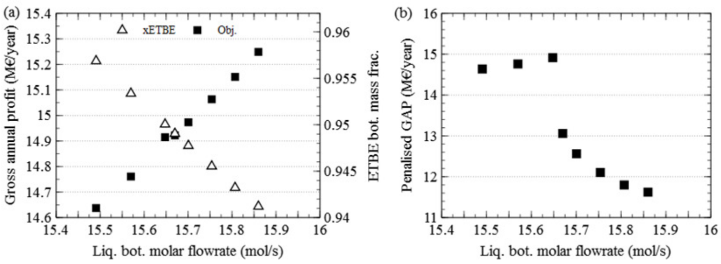


Fig. 4 – Sensitivity analysis for the liquid bottom molar flowrate. (a) Variation of the objective function with no penalty and ETBE bottom mass fraction. (b) Variation of the objective function with penalty.

Conclusions

- Even though GAs have been previously used to solve RD design problems, it is shown that the simpler PSO algorithm is also a promising tool (Fig .3)
- The configuration obtained by the PSO algorithm is the optimum, as shown by the sensitivity analysis (Fig. 4)
- The proposed methodology is adequate to solve this problem

References

[1] Kirk-Othmer Encyclopedia of Chemical Technology (5th Ed.), Vol. 10, New York, United States, John Wiley & Sons (2005).

[2] L Domingues, C I C Pinheiro, N M C Oliveira, J Fernandes, A Vilelas, *Ind. Eng. Chem. Res.*, vol. 51 (2012) pp. 15018–15031.

Acknowledgements

The author Luís Domingues thanks the financial support granted by Fundação para a Ciência e Tecnologia through Grant No. SFRH/BD/60668/2009.
The authors thank Repsol Polímeros S.A., Sines, Portugal