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An evolutionary approach for multi-objective dynamic optimization applied to middle vessel batch distillation

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ABSTRACT

In this paper, a new approach is presented to perform multi-objective dynamic optimizations of novel batch distillation utilizing an evolutionary algorithm. The contribution is divided into two major parts. First, the development of an efficient hybrid evolutionary algorithm covering multi-objective mixed integer dynamic optimization problems is presented. The efficiency of the optimization solver is proven by several complex test problems. Second, the application of the algorithm is shown by the optimization of a middle vessel batch distillation. The challenging non-linear dynamic model, which takes the start-up phase into account, is solved in Aspen Custom Modeler. It could be proven that the proposed evolutionary algorithm can be applied to complex mathematical problems. Likewise the algorithm was found to successfully handle the optimization of middle a vessel batch distillation. The results show the feasibility of the proposed methodology and a significant increase in profitability of the process.

1. Introduction

For the task of separating low quantities of high value-added products in specialty and fine chemistry novel batch distillation columns have been proposed and investigated in the last decade, in particular, the multi-vessel batch distillation (MBD), which can be considered as a superstructure of all batch distillation configurations. It consists of a reboiler, a total condenser, a distillate receiver, N-1 thermally coupled column sections and N-2 intermediate vessels where N indicates the number of separated fractions. From a practical and theoretical point of view, it is generally recommended to operate the column with infinite reboil and reflux ratio (Furlonge, Pantelides, & Sørensen, 1999). The products are simultaneously collected in associated vessels applying an appropriate process control strategy, so that no off-cuts have to be reprocessed. A MBD with one intermediate vessel, namely the middle vessel batch distillation (MVBD), which is focus of this contribution, is illustrated in Fig. 1.

MBD and MVBD has been subject to many investigations, whereas primarily process control strategies have been proposed (Barolo, Guarise, Ribon, Rienzi, & Trotta, 1996; Hasebe, Kurooka, & Hashimoto, 1995; Wittgens, Litto, Sørensen, & Skogestad, 1996). Hasebe, Noda, and Hashimoto (1999) as well as Furlonge et al. (1999) performed dynamic optimization studies with respect to a minimum energy consumption. Low and Sørensen (2003, 2005) carried out single objective optimization (SOO) studies to optimize process design and operating parameters of a MBD simultaneously. However, the weighting of the single targets within the objective function is always difficult to handle in the design phase of a process. Moreover, the optimization results in one single solution on which a decision has to be made. Using multi-objective optimization (MOO), it would be possible to pick the best solution for an actual problem considering non-mathematical decision variables. Recently, Barakat, Fraga, and Sørensen (2006) presented results of MOO studies applied to conventional batch distillation. To the best of our knowledge, no publication deals with the MOO of multi-vessel batch distillation. Thus, the aim of this contribution is to optimize the dynamic process of a MVBD in terms of operation costs while simultaneously consider investment costs.

A formulation of such kind of problem will lead to a mixed integer non-linear programming (MINLP) problem. Different approaches can be found in the open literature to solve MINLP problems, for example *Branch and Bound* methods or *Outer Approximation* (Biegler & Grossmann, 2004; Floudas, Akrotirianakis, Caratzoulas, Meyer, & Kallrath, 2005). Most of these established methods are only able to handle one single objective function and can only supply one solution each run. For these methods management of multiple targets results in an *a priori* weighting of the single objectives and formulation of a combined objective function that will be solved. Such approach is called *Weighted Sum Method* and is the simplest approach for solving MOO problems (Deb, 2004). To obtain more then one solution weights have to be changed and optimization have to be repeated several times. Although the method is intuitive and easy to use it holds the risk not to be able to find

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Nomenclature

A	surface area, refers to the heat transfer (m^2)
C_1	cost factors for consideration of installation, maintenance . . . (–)
C_2	costs of packed column (€ m^{-1})
C_3	costs of total condenser (€)
C_4	costs of falling film evaporator (€)
C_5	costs for steam (€ t^{-1})
c_p	heat capacity (J (kg K)$^{-1}$)
CR	crossover probability (–)
D	diameter (m)
d	Euclidean distance (–)
f	objective function (–)
F	scaling factor (–)
F_{max}	maximum possible fitness (–)
F'	reduced fitness (–)
F_V	vapor load (Pa$^{0.5}$)
g	inequality constraint (–)
G_{max}	maximum number of generations (–)
h	dynamic process model (–)
H	enthalpy (J)
h	specific enthalpy (J kg^{-1})
HETP	height equivalent to the theoretical plate (m)
HU_{max}	maximum liquid hold-up (ml)
I	individual
IC	investment costs (€)
k	overall heat transfer coefficient (W m^{-2} K^{-1})
K	vapor–liquid equilibrium constant (–)
L	liquid flow (kg h^{-1})
m	mass (kg)
M	dimension of genome (–)
n	recovery period (a)
N	number of fractions (–)
N_{Pop}	population size (–)
N_{th}	number of theoretical stages (–)
nc	niche count (–)
OC	operation costs (€)
p	pressure (Pa)
P	population (–)
Q	heat duty (kW)
r	randomly selected individual (–)
R	reboil/reflux ratio (–)
S	split ratio (–)
sh	sharing function value (–)
t	time (h)
T	temperature (°C)
T_A	annual production time (h a^{-1})
t_B	batch time (h)
t_S	set-up time (h)
$\underline{u}_d$	design variables
$\underline{u}_o$	operating variables
V	vapor flow (kg h^{-1})
V	Volume (m^3)
w	mass fraction (kg kg^{-1})
x	gene/parameter
x	liquid mass fraction (kg kg^{-1})
$\underline{x}$	state variables
$\dot{\underline{x}}$	time-dependent state variables
y	vapor mass fraction (kg kg^{-1})

Greek letters

Δh_V	enthalpy of evaporation (kJ kg^{-1})
σ_{share}	maximum considered distance (–)
μ	population size (–)
$\mu(\Omega_i)$	number of individuals in front i (–)
Ω	non-constrain-dominated front (–)

Indices

B	bottom
col	column
cond	condenser
D	distillate
feed	feed
i, j	individual counter
init	initial
internals	internals
j	tray counter
l	lower bound
L	liquid
loss	loss
m	gene counter
max	maximum
min	minimum
packings	column packings
reb	reboiler
shell	shell
steam	steam
stage	stage
u	upper bound
V	vapor

Abbreviations

DE	differential evolution
EA	evolutionary algorithm
ES	evolution strategy
GA	genetic algorithm
MBD	multi-vessel batch distillation
MDE	modified differential evolution
MIDO	mixed integer dynamic optimization
MINLP	mixed integer non-linear programming
MOO	multi-objective optimization
MVBD	middle vessel batch distillation
ncsMDE	non-constrain-dominated sorting modified differential evolution
NRV	noisy random vector
NSGA	non-dominated sorting genetic algorithm
PDE	pareto-frontier differential evolution
rGA	real-valued genetic algorithm
SOO	single objective optimization
TV	trial vector
VEGA	vector evaluated GA

a well distributed front of optimal tradeoffs (pareto optimal front). This is due to the fact that not all different weight vectors must correspond to different solutions and that two very similar sets of parameters may correspond to solutions in different regions regarding objective space. As a side effect the computational complexity of the weighted sum approach is quite high due to the large number of optimization runs. The only promising method known to solve MOO problems in one optimization run is to make use of stochastic optimization algorithms, in particular, evolutionary algorithms (EA). Many EAs can be found in the open literature, for example, the so-called vector evaluated genetic algorithm (VEGA) (Schaffer, 1985), the non-dominated sorting genetic algorithm (NSGA) (Srinivas & Deb, 1994) or the pareto-frontier differential evolution algorithm (PDE) (Abbass, Saker, & Newton, 2001). Yet no standard is available