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Improvements in surrogate models for process synthesis. Application to water network system design

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ABSTRACT

High accuracy models can be obtained by using different types of surrogate models that accurately approximate equipment phenomenological models and can be used in synthesis problems, leading to faster and more precise solutions. Two types of surrogate models are used to approximate equipment phenomenological models: polynomial and neural network-based. In some cases, these surrogate models are not able to represent more complex equipment. An original methodology to reformulate these models using equations from shortcut equipment design is proposed. A medium-size case study involving fifteen units is presented. The synthesis problem is solved in a short computational time, leading many local solutions. Since several local optima objective function values are very close to each other, the choice of the best configuration among those found should be done qualitatively, because the differences among the objective function values are not significant if compared to the accuracy of equipment cost correlations in the literature.

1. Introduction

Several methodologies were developed for the synthesis and optimization of WN (water networks), which can be divided into: mathematical programming (Faria & Bagajewicz, 2009; Galan & Grossmann, 1998; Takama, Kuriyama, Shiroko, & Umeda, 1980a); conceptual design (Freitas, Costa, & Boaventura, 2000) and pinch analysis (Kuo & Smith, 1997; Wang & Smith, 1994). The first technique shows more advantages when compared to the others, because it takes into account all the possible system configurations. The second one, conceptual design technique, is based on the flow sheet built as from a critical equipment, following sequentially through the other ones and the last, pinch analysis, is based on the thermodynamical limitation of mass transfer.

The research about synthesis and optimization of wastewater networks started with Takama, Kuriyama, Shiroko, and Umeda (1980b). In this work, the authors aimed to decrease the general water consumption in a refinery by segregation and integration of wastewater process streams, modeling the wastewater allocation problem as a superstructure.

Although the equipment models employed in this case are simple, the large number of both nonlinear terms and design possibilities (of the superstructure model), lead to difficulties to solve the equation system. To address this problem, Takama and coworker applied both penalty function and structure reduction step to obtain a viable solution.

The WN research based on mathematical programming approach was continued by Alva-Argáez, Kokossis, and Smith (1998) who modified the first model developed by Takama et al. (1980b), assigning a binary variable to each possible stream connection. Furthermore, they fixed the outlet stream concentrations of all the equipment, converting the initial NLP (nonlinear programming) into an MILP (mixer integer linear programming).

Galan and Grossmann (1998) developed an MINLP (mixer integer nonlinear programming) for the WN problem. Moreover, they created a heuristic methodology to find the global optimal solution for both the NLP originally modeled by Takama et al. (1980b) and the new WN problem modeled as an MINLP proposed by them. Huang, Chang, Ling, and Chang (1999) solved a refinery wastewater network problem with equipment models, slightly more sophisticated than the previous ones, as it considered water loss in the equipment models.

After 2000, the works in this area were oriented to find the global optimal solution of NLPs and MINLPs, created in the superstructure modeling (Bergamini, Aguirre, & Grossmann, 2005; Bergamini, Grossmann, Scenna, & Aguirre, 2008; Castro, Teles, & Novais, 2008; Chang & Li, 2005; Chang, Li, & Liou, 2009; Faria & Bagajewicz, 2011; Gabriel & El-Halwagi, 2005; Hernandez, Castellanos, & Zamora, 2004; Karuppiah & Grossmann, 2006; Lee & Grossmann, 2003, 2001; Li & Chang, 2007; Meyer & Floudas, 2006; Teles, Castro, & Novais, 2009; Ahmetović and Grossmann, 2011).

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List of variables

y	vector of dependent variables
bv	binary variable
θ	polynomial model parameters
x	independent variables
m	number of independent variables
t	number of terms in the polynomial model
n	number of neurons in the second layer
LW	weight matrix of third layer
IW	weight matrix of the second layer
$b2$	bias vector of the second layer
$b3$	bias vector of third layer
Fw	water flow rate
Tw	water temperature
A_{fr}	cross section area
Fa	air flow rate
L_{fi}	fill height
Z	contaminant concentration
Zin	contaminant concentration of inlet stream
$Zout$	contaminant concentration of outlet stream
NTU	number of theoretical units
MRR	molar reflux ration
T_{press}	column top pressure
$Fvap$	steam feed flow rate
H	column height
V	steam molar flow rate inside the column
L	liquid molar flow rate inside the column
S	stripper factor
dF	effluent loss
dT	difference between the inlet and outlet stream temperature
TC	heat exchanger
TAC	total annualized cost

Subscript

SD	stripper without reboiler
SR	stripper with reboiler
NaCl	salt
Oil	organic compounds
H_2S	hydrogen sulfide
NH_3	ammonia
in	inlet
out	outlet
B	column bottom
T	column top
st	stripper cost
ref	refrigeration cost
sep	oil separator cost
pur	purification cost
plant	discharge to plant wastewater treatment unit cost
site	discharge to site wastewater treatment unit cost
EI	energy integration
SH	steam heating
max	upper bound
min	lower bound

Superscript

fill	fill type (splash, trickle or film)
ct	column type (with or without reboiler)

Jeżowski (2010) produced the most recent review in this area, with 264 notes on papers about energy and mass integration for water consumption reduction. The author suggests that more realistic models should be used to represent equipment in the model superstructure (for example, including construction variables in equipment models) and that temperature should be considered as a variable in the equipment modeling, for a more realistic analysis of the system behavior.

These two crucial points need to be considered in WN equipment models. However, the use of phenomenological models in an optimization platform such as GAMS would be unfeasible due to high computational time and technical difficulties to program thermodynamic modules with similar performance to the property packages of commercial simulators.

High accuracy models that do not require large computational time can be obtained by using different types of surrogate models, which are able to approximate the equipment phenomenological models. These models can be employed in the solution of the synthesis problem in an optimization platform, leading to more precise solutions. Despite their great versatility, there are some complex problems that cannot be represented by surrogate models in a straightforward way due to their inherent nonlinearity. We here show that surrogate models inspired by established shortcut models can be used, expanding the possibilities of process synthesis based on superstructure optimization.

Surrogate models design and the methodology to build them is presented in Section 2. In Section 3, we show a simple implementation of surrogate models to represent equipment for wastewater network synthesis. In the fourth section, we present an example with more complex equipment, for which ordinary surrogate model fit fails, and we show a strategy to solve using a new hybrid surrogate model based on established shortcut models. The approach is applied to a complex case study of a wastewater network synthesis. Finally, the results of this case study are extremely interesting because they illustrate the non-convex nature of process synthesis. A given number of local solutions are obtained that are the same in essence, but depending on the accuracy of the surrogate model approximation, they are obtained in a different order.

2. Surrogate models

Surrogate models, meta-models or response surface models are black box models that can approximate the behavior of complex phenomenological models (within a limited range), using low computational time. These models do not take into account the process phenomenology, so that their equations are only a correlation of the outlet variables with respect to the inlet variables.

Optimization based on surrogate models can be represented by the following steps:

- A sample set is obtained by designing a set of experiments within the operational range of the independent variables chosen.
- The phenomenological model is simulated using the sample set as an input, providing outlet points set.
- The sample points set and the outlet points set are used to fit and to validate the surrogate model.
- Finally, the surrogate model structure is optimized.

There are several types of surrogate models in the literature, such as: polynomial, Kriging interpolation, neural network and splines. These models can be divided into two categories: interpolating models, as the Kriging interpolation and splines, in which the response surface comprises all the sample points; and non-interpolating models, such as polynomial and neural networks, which minimize the sum of the error between sample points and the response surface (Müller & Piché, 2010). However, a given type of surrogate model is not able to solve all the problems,