

# New MINLP Formulation for the Multiperiod Pooling Problem

Pedro M. Castro

Centro de Matemática Aplicações Fundamentais e Investigação Operacional, Faculdade de Ciências, Universidade de Lisboa, 1749-016 Lisboa, Portugal

DOI 10.1002/aic.15018

Published online September 3, 2015 in Wiley Online Library (wileyonlinelibrary.com)

*The modeling of blending tank operations in petroleum refineries for the most profitable production of liquid fuels in a context of time-varying supply and demand is addressed. A new mixed-integer nonlinear programming formulation is proposed that using individual flows and split fractions as key model variables leads to a different set of nonconvex bilinear terms compared with the original work of Kolodziej et al. These are better handled by decomposition algorithms that divide the problem into integer and nonlinear components as well as by commercial solvers. In fact, BARON and GloMIQO can solve to global optimality all problems resulting from the new formulation and test problems from the literature. A tailored global optimization algorithm working with a tight mixed-integer linear relaxation from multiparametric disaggregation achieves a similar performance.* © 2015 American Institute of Chemical Engineers *AICHE J*, 61: 3728–3738, 2015

**Keywords:** mathematical modeling, optimization, scheduling, process networks, mixed-integer quadratically constrained problem

## Introduction

Finding the most profitable blends of different distilled fractions so as to meet technical and environmental regulations is a problem of great importance in petroleum refineries. It was first formulated by Haverly<sup>1</sup> and became known as the pooling problem. The pools represent blending tanks whose content, generated from the mixing of liquid fuels with known properties and used to supply the final products, is going to be determined by the optimization. Due to an unknown inventory of different fuels and multiple outlet streams, the pooling problem is of the nonlinear (NLP) type featuring nonconvex bilinear terms that are known to cause difficulties to gradient-based solvers. In contrast, stream mixing in a process network<sup>2</sup> can be modeled linearly<sup>3</sup> and so can the removal from a tank with known composition<sup>4</sup> (single fuel).

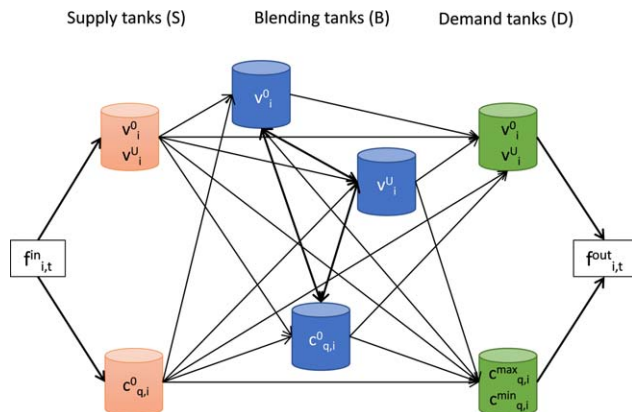
Albeit simple to pose, a few formulations have been proposed for the pooling problem. The p-formulation<sup>1</sup> features total flows and compositions as model variables. The q-formulation of Ben-Tal et al.<sup>5</sup> keeps the total flows but replaces pool compositions with the mass fractions of fuels making the blend, which add up to one. Tawarmalani and Sahinidis<sup>6</sup> combined the two into a pq-formulation that included redundant constraints for strengthening the formulation. More recently, Alfaki and Haugland<sup>7</sup> proposed the tp-formulation with variables for the proportion of the pool being sent to each final product, again summing one. As the quality of the McCormick relaxation<sup>8</sup> from the tp-formulation (compared with pq) is sometimes better but sometimes worse, the authors came up with the stp-formulation featuring source and terminal proportions, which is at least as tight as the others.

In the generalized pooling problem,<sup>9</sup> interpool links are permitted and binary variables are added to the formulation to ensure that flow rates are between given lower and upper bounds, leading to a mixed-integer nonlinear problem (MINLP). The extended pooling problem<sup>10</sup> incorporates the nonconvex emission model of the US Environmental Protection Agency (EPA)<sup>11</sup> and associated legislative bounds into the constraint set.<sup>12</sup> All these are aimed at steady-state operation. In reality, however, supply and demand vary with time, resulting in a multiperiod pooling problem<sup>13</sup> (Lotero et al., An MILP-MINLP decomposition method for the global optimization of a source based model of the multiperiod blending problem, Submitted) where model entities gain a time index, and tank capacity and logistic constraints (concerning the movement of materials into and out of tanks) need to be enforced.

Due to the static nature of the time intervals, the operational part of the multiperiod pooling problem is more of a planning than a scheduling problem. The crude oil unloading and inventory management problem<sup>14–22</sup> is closely related but more detailed in the sense that the duration of the time intervals is going to be determined by the optimization, taking into account the arrival times of marine vessels and the different transfer rates between tanks so as to minimize operating cost. This includes sea waiting and harboring costs that are a function of the time the vessel takes to complete these tasks, as well as inventory costs, which are computed as the sum over all intervals of the product of the average inventory by the duration of the time interval (another source of bilinear terms when using a continuous-time formulation<sup>4</sup>).

In recent work,<sup>4</sup> we have shown that a Resource-Task Network<sup>23</sup> continuous-time formulation<sup>24</sup> can effectively capture the most important scheduling constraints of crude oil blending and be solved very efficiently by commercial global optimization solvers. The material resources are the different

Correspondence concerning this article should be addressed to P. M. Castro at pmcastro@fc.ul.pt.



**Figure 1. Network configuration of multiperiod pooling problem.**

Note that supply tanks can be connected to both blending and demand tanks. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]

crudes and their location as they move from the marine vessels up to the distillation columns, with the contents of a tank consisting of multiple crudes rather than a single resource of unknown composition. The challenge is then to enforce that a tank's outlet stream has the exact same composition of the blend inside the tank, which is accomplished through bilinear constraints featuring split fraction variables. These are similar to the ones used in the tp-formulation of Alfaki and Haugland,<sup>7</sup> with the difference being that the sum of the split fraction over all possible outlet streams does not add to one as some inventory may be left in the tank to be used in subsequent time periods, something that is not relevant in the steady-state pooling problem. The main novelty of this work is thus to define the liquid fuels initially present in the system (or supplied later) as new model entities and propose a new formulation with split fraction variables that keeps track of their location through time.

The multiperiod pooling problem can be classified as a mixed-integer quadratically constrained problem in which binary variables appear linearly in the constraints. Commercial global optimization solvers<sup>25–27</sup> rely on a linear or mixed-integer linear programming (MILP) relaxation of the bilinear terms. The latter type can be considerably tighter, something that is critical to ensure fast convergence. There are essentially two types of MILP relaxations for bilinear problems, originating from: (1) piecewise McCormick envelopes<sup>28,29</sup> and (2) multiparametric disaggregation.<sup>30,31</sup> Piecewise McCormick envelopes work by partitioning the domain of one of the variables of each bilinear term, which can be done in a variety of ways.<sup>32–35</sup> Multiparametric disaggregation is conceptually different as it discretizes<sup>30</sup> the domain to a certain accuracy level, ultimately leading to a rigorous relaxation after the addition of a slack variable to achieve a continuous domain.<sup>31</sup> More importantly, it scales much more favorably with increasing accuracy resulting in a computational performance that is often orders of magnitude faster.<sup>31,36</sup> For the specific case of the crude oil scheduling problem, it was shown<sup>4</sup> capable of reducing the optimality gap by orders of magnitude compared with commercial solvers and hence is considered again in this article.

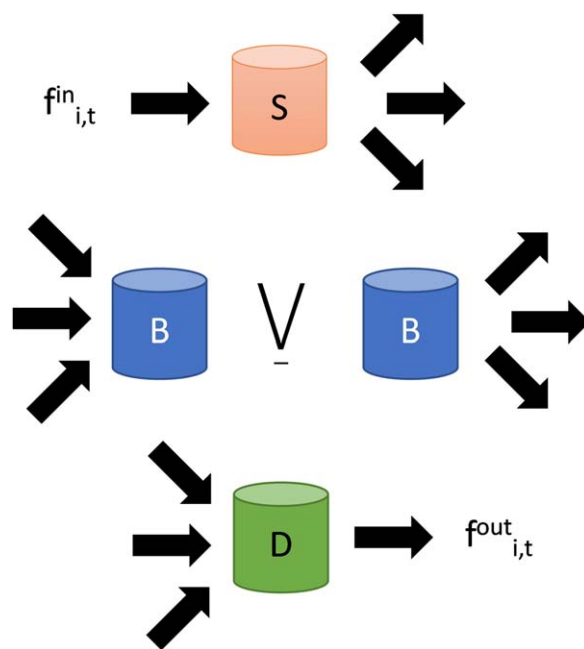
## Problem Statement

The multiperiod pooling problem addressed in this article is taken from Kolodziej et al.<sup>13</sup> and involves the production of

liquid fuels in petroleum refineries by blending streams originating from different tanks. Unlike the traditional pooling problem that is assumed to operate at steady state, in the multiperiod problem, supply and demand are specified as a function of time and the inventory in each tank is allowed to vary from one time period to the next so as to obtain the most profitable products.

Let  $i \in I$  represent a tank belonging to the subset of supply  $S$ , blending  $B$ , or demand tanks  $D$  ( $I = S \cup B \cup D$ ), see Figure 1. Supply tanks  $i \in S$  are characterized by mass  $f_{i,t}^{in}$  (kg) arriving during the different planning periods  $t \in T$  being assumed that a single liquid fuel is involved. In other words, the properties (called qualities  $q \in Q$ ) of the liquid mixture inside the tank are constant with time and so their values are equal to the initial compositions  $c_{q,i}^0$  (mass%). Because of this, supply tanks are allowed to have simultaneous inlet and outlet transfers. In contrast, the composition of blending tanks  $B$  will vary with time and so there can either be flow in or out, which is known as standing-gage operation<sup>14</sup> (Figure 2). Demand tanks  $D$  also have varying compositions but are modeled in a simpler way. Instead of keeping track of compositions over time (not possible as the problem data does not feature initial compositions<sup>13</sup>), demand tanks have lower  $c_{q,i}^{\min}$  and upper bounds  $c_{q,i}^{\max}$  (mass%) on compositions that are enforced by ensuring that all input streams from supply or blending tanks have compositions within such values. As a result, demand tanks, like supply tanks, can also have simultaneous inlet and outlet transfers.

The transfer of material between tanks  $i$  and  $i'$  is charged a fixed  $cs_{i,i'}^{fx}$  (\$) and a variable cost  $cs_{i,i'}^{vr}$  (\$/kg) and must lie within  $f_{i,i'}^{\min}$  and  $f_{i,i'}^{\max}$  (kg). If at least one parameter is positive, then the pair of tanks is connected, that is, tank  $i$  can feed  $i'$  ( $i \in I_{i'}$ ). Material transfer from supply tank  $i$  has a negative value  $p_i$  while the transfer to demand tank  $i'$  has a positive value  $p_{i'}$  (\$/



**Figure 2. Supply and demand tanks can have simultaneous flow in and out contrary to blending tanks.**

All of them can have multiple input/output streams. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]

kg). Other tank related parameters include initial inventory  $v_i^0$  (kg), maximum capacity  $v_i^{\max}$  (kg), and, in the case of demand tanks, removed mass  $f_{i,t}^{\text{out}}$  (kg).

### Remarks

In general, all system tanks should be modeled as blending tanks with given initial, minimum, and maximum compositions, and subject to the constraint of either flow in or flow out (to have reasonably accurate material balances). In particular, the assumption of all input streams to a demand tank being within its composition bounds may lead to a suboptimal solution as the real constraint is for the mix to be within the bounds, which may be achieved by incorporating small amounts of low-cost, low-quality (high composition) fuels. The impact of replacing the assumption by the real constraint is evaluated toward the end of the computational results section.

### MINLP Model with Total Flows and Composition Variables

The mathematical formulation proposed by Kolodziej et al.<sup>13</sup> for solving the multiperiod pooling problem is perhaps the most intuitive. Total flows between tanks  $F_{i,i',t}$  (kg) and compositions  $C_{q,i,t}$  (mass%) are the key model variables, a feature shared with the original p-formulation proposed by Haverly<sup>1</sup> for the steady-state pooling problem and with most models for process networks.<sup>9,29,37–39</sup> The remaining set of nonnegative continuous variables is the total amount inside the tanks  $V_{i,t}$  (kg), while binary variables  $Y_{i,i',t}$  indicate the existence of flow between tanks  $i$  and  $i'$  during interval  $t$ .

The total mass balance states that the amount inside tank  $i$  at the end of interval  $t$  is equal to the amount at the end of  $t-1$  (or to the initial inventory  $v_i^0$  if  $t=1$ ) plus incoming flows from all tanks  $i'$  feeding  $i$  minus outgoing flows, Eq. 1

$$V_{i,t} = v_i^0|_{t=1} + V_{i,t-1}|_{t>1} + f_{i,t}^{\text{in}} + \sum_{i' \in I_i} F_{i',i,t} - f_{i,t}^{\text{out}} - \sum_{i' \in I_{i'}} F_{i,i',t} \quad \forall i, t \quad (1)$$

The mass balance for each individual quality  $q$  follows the same principle but is a little more difficult to understand due to the dynamics involved, see Eq. 2. If the input flow comes from a source tank, its composition is constant and equal to the initial value  $c_{q,i}^0$ . If the input flow comes from a blending tank, the composition to consider at  $t=1$  is also the initial one. For the remaining intervals, the composition is the one at  $t-1$  as flows arriving to the tank at the end of  $t$  started to be pumped at  $t-1$ . Note the appearance of two different types of bilinear terms,  $C_{q,i,t}V_{i,t}$ , and  $C_{q,i,t-1}F_{i,i',t}$ , and that the constraint only needs to be applied to blending tanks

$$C_{q,i,t}V_{i,t} = \left(c_{q,i}^0 v_i^0\right)|_{t=1} + (C_{q,i,t-1}V_{i,t-1})|_{t>1} + \sum_{i' \in I_i \cap S} c_{q,i'}^0 F_{i',i,t} + \sum_{i' \in I_i \cap B} \left[ \left(c_{q,i'}^0|_{t=1} + C_{q,i',t-1}|_{t>1}\right) F_{i',i,t} \right] - \sum_{i' \in I_{i'}} \left[ \left(c_{q,i}^0|_{t=1} + C_{q,i,t-1}|_{t>1}\right) F_{i,i',t} \right] \quad \forall q, i \in B, t \quad (2)$$

Flow to a demand tank  $i'$  is allowed only if the composition is within the tank's given lower and upper bounds. This can be written as a disjunction (Eqs. 3 and 4) and reformulated into Eqs. 5 and 6. As the constraint inside the left term in Eq. 3 involves only parameters, it suffices to multiply the binary variable by all terms to generate the MILP constraint in Eq. 5

(the binary variables could alternatively be eliminated as a preprocessing step). In the actual implementation, Kolodziej et al.<sup>13</sup> actually used a big-M constraint similar to Eq. 6

$$\left[ \begin{array}{c} Y_{i,i',t} \\ c_{q,i'}^{\min} \leq c_{q,i}^0 \leq c_{q,i'}^{\max} \end{array} \right] \bigvee \left[ \begin{array}{c} -Y_{i,i',t} \\ c_{q,i}^0 \geq 0 \end{array} \right] \quad \forall q, i' \in D, \quad (3)$$

$$i \in I_{i'}, (i \in S, t \in T \vee i \in B, t=1)$$

$$\left[ \begin{array}{c} Y_{i,i',t} \\ c_{q,i'}^{\min} \leq C_{q,i,t-1} \leq c_{q,i'}^{\max} \end{array} \right] \bigvee \left[ \begin{array}{c} -Y_{i,i',t} \\ C_{q,i,t-1} \geq 0 \end{array} \right] \quad \forall q, i' \in D, \quad (4)$$

$$i \in I_{i'} \cap B, t > 1$$

$$c_{q,i'}^{\min} Y_{i,i',t} \leq c_{q,i}^0 Y_{i,i',t} \leq c_{q,i'}^{\max} Y_{i,i',t} \quad \forall q, i' \in D, \quad (5)$$

$$i \in I_{i'}, (i \in S, t \in T \vee i \in B, t=1)$$

$$c_{q,i'}^{\min} - M(1 - Y_{i,i',t}) \leq C_{q,i,t-1} \leq c_{q,i'}^{\max} + M(1 - Y_{i,i',t}) \quad \forall q, i' \in D, \quad (6)$$

$$i \in I_{i'} \cap B, t > 1$$

The remaining constraints, respectively, limit the flow rates between tanks to the given intervals, ensure no simultaneous flow in and out of blending tanks and ensure that inventory does not exceed maximum capacity, Eqs. 7–9

$$f_{i,i'}^{\min} Y_{i,i',t} \leq F_{i,i',t} \leq f_{i,i'}^{\max} Y_{i,i',t} \quad \forall i', i \in I_{i'}, t \quad (7)$$

$$Y_{i',i,t} + Y_{i,i',t} \leq 1 \quad \forall i', i \in I_{i'} \cap B, i' \in I_i, t \quad (8)$$

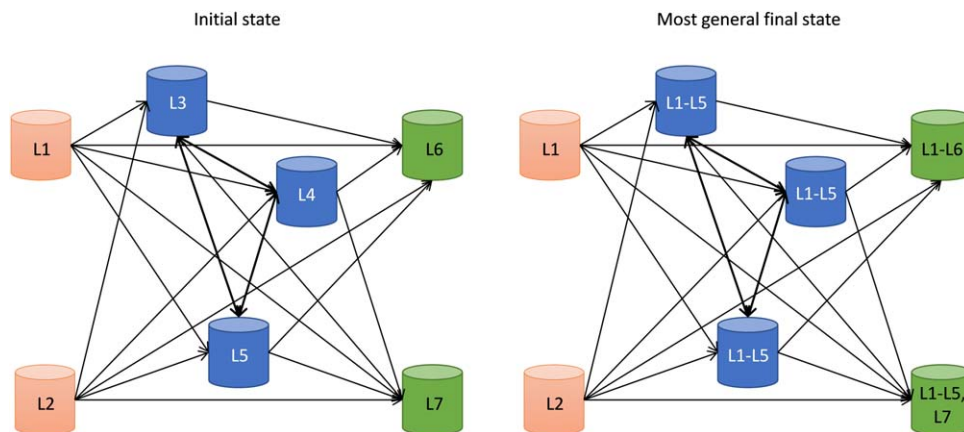
$$V_{i,t} \leq v_i^{\max} \quad \forall i, t \quad (9)$$

The mixed-integer nonlinear programming (MINLP) model is complete with the objective function in Eq. 10 that maximizes the profit made from delivering fuel to demand tanks minus the costs associated with supply flows and pumping the fuel between tanks

$$\max \sum_{i'} \sum_{i \in I_{i'}} \sum_t \left[ (p_i + p_{i'} - c_{i,i'}^{\text{vr}}) F_{i,i',t} - c_{i,i'}^{\text{fx}} Y_{i,i',t} \right] \quad (10)$$

### New MINLP Model with Individual Flows and Split Fraction Variables

The new formulation uses individual flows and split fractions as the key model variables. Our recent results<sup>4</sup> for crude oil blending and scheduling with a continuous-time formulation have shown that it is a choice leading to very good computational performance. We now move away from the Resource-Task Network<sup>23</sup> nomenclature to present a model that is easier to understand, something that is possible due to the discrete-time nature of the current problem, with time periods that are known *a priori* (for a review of the alternative time representation concepts see Harjunkoski et al.<sup>40</sup>). Motivated by the need to avoid numerical irregularities, Furman et al.<sup>18</sup> were the firsts to relate the remaining content of a tank with its outlet streams through a nonlinear constraint, an approach that continued in subsequent work.<sup>20,41</sup> However, these works did not explicitly define a split fraction variable and used individual flows, total flows, and tank volumes, leading to the appearance of more bilinear terms. In steady-state problems, the split fraction has been used to relate the outlet of a stream to the total flow of all outlet streams from a node. Examples can be found in the work of Galan and Grossmann<sup>3</sup> for process networks and in the recent tp-formulation of Alfaki and Haugland<sup>7</sup> for the pooling problem.



**Figure 3. Correspondence between liquid fuels and demand tanks.**

On the left, the initial blend inside a tank defines a liquid fuel. On the right, and given enough time periods, all fuels initially present in supply and blending tanks may end up in a blending or demand tank (assuming full connectivity between blending tanks). [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]

Let  $l \in L$  be a liquid fuel present in the system. Note that for the given problem definition  $L$  can be seen as an alias of  $I$  but in cases with external input streams featuring time-varying compositions it will hold more elements than the number of tanks. Then, let  $L_i$  be the subset holding the liquid fuels that can appear at some point in time in tank  $i$  (if needed, the time index  $t$  can be added to reduce the number of model entities). Figure 3 shows how to define these sets for a generic problem.

An individual flow thus refers to the flow of liquid fuel  $l$  between tanks  $i$  and  $i'$  during interval  $t$ , being represented by continuous variable  $F_{l,i,i',t}$  (kg). Unlike the external input to a supply tank that features a single fuel, external outputs from demand tanks will typically consist of a mixed fuel, leading to variables  $F_{l,i,t}^{\text{out}}$  (kg). The amount inside a tank is also fuel dependent:  $V_{l,i,t}$  (kg). Variables  $X_{i,i',t} \in [0, 1]$  then hold the fraction of the contents of tank  $i$  at time  $t - 1$  leaving for tank  $i'$  during interval  $t$ . Finally, binary variables  $Y_{i,i',t}$  are shared with the previous model.

The mass balances are conceptually similar to Eq. 1 but are now written for every liquid fuel. Note that in Eq. 11, parameter  $v_{l,i}^0$  is equal to  $v_i^0$  for the single fuel initially present in tank  $i$  (recall Figure 3) and zero otherwise. The same is true for the relation between  $f_{l,i,t}^{\text{in}}$  and  $f_{i,t}^{\text{in}}$

$$V_{l,i,t} = v_{l,i}^0 |_{t=1} + V_{l,i,t-1} |_{t>1} + f_{l,i,t}^{\text{in}} + \sum_{i' \in I_i: l \in L_{i'}} F_{l,i',t} - F_{l,i,t}^{\text{out}} |_{i \in D} - \sum_{i' \in I_i'} F_{l,i,i',t} \quad \forall i, l \in L_i, t \quad (11)$$

Equation 12 states that the sum of external outlet flows must be equal to the given demands. Transfer flows are subject to given bounds, Eq. 13, and the total amount inside a tank must not exceed its capacity, Eq. 14

$$f_{i,t}^{\text{out}} = \sum_{l \in L_i} F_{l,i,t}^{\text{out}} \quad \forall i \in D, t \quad (12)$$

$$f_{i,i',t}^{\text{min}} Y_{i,i',t} \leq \sum_{l \in L_i} F_{l,i,i',t} \leq f_{i,i',t}^{\text{max}} Y_{i,i',t} \quad \forall i', i \in I_i', t \quad (13)$$

$$\sum_{l \in L_i} V_{l,i,t} \leq v_i^{\text{max}} \quad \forall i, t \quad (14)$$

Eqs. 5 and 8 are also part of the model. In contrast, Eq. 6 needs to be changed as we no longer have composition variables. Let parameter  $c_{q,l}$  (mass%) represent the composition of

fuel  $l$  in quality  $q$ , which is computed from the initial compositions  $c_{q,i}^0$  and the 1:1 correspondence between fuels and tanks. By adding the product of the individual amounts by the fuel composition and dividing by the total amount, one can calculate the composition inside the blending tank. This can then be subject to the lower and upper bounds of the destination tank composition, leading to Eq. 15

$$\begin{aligned} c_{q,i'}^{\text{min}} \sum_{l \in L_i} V_{l,i,t-1} - M(1 - Y_{i,i',t}) \\ \leq \sum_{l \in L_i} c_{q,l} V_{l,i,t-1} \leq c_{q,i'}^{\text{max}} \sum_{l \in L_i} V_{l,i,t-1} \\ + M(1 - Y_{i,i',t}) \quad \forall q, i' \in D, i \in I_i' \cap B, t > 1 \end{aligned} \quad (15)$$

The nonconvex bilinear constraint in Eq. 16 defines the split fraction between a tank's contents and one of its outlet streams. This constraint is written for blending tanks only, meaning that the outlet stream from demand tanks may feature a single liquid fuel even if there are multiple fuels inside (note that we are not concerned with the accurate modeling of demand tanks as Eqs. 5 and 15 already ensure the right composition, see remarks in problem statement section). Furthermore, as flows during  $t=1$  move the tank's initial blend, which by definition consists of a single liquid fuel, it is sufficient to write it for  $t > 1$

$$F_{l,i,i',t} = X_{i,i',t} V_{l,i,t-1} \quad \forall i', i \in I_i' \cap B, l \in L_i, t > 1 \quad (16)$$

The last constraint of the MINLP formulation is the objective function in Eq. 17

$$\max \sum_{i'} \sum_{i \in I_i'} \sum_t \left[ (p_i + p_{i'} - c_{i,i'}^{\text{vr}}) \sum_{l \in L_i} F_{l,i,i',t} - c_{i,i'}^{\text{fx}} Y_{i,i',t} \right] \quad (17)$$

### MILP Relaxation with McCormick Envelopes

A rigorous upper bound on the optimal solution to the multiperiod pooling problem can be obtained by solving a MILP relaxation of the nonconvex MINLP maximization problem. The standard approach is to replace bilinear term  $X_{i,i',t} V_{l,i,t-1}$  with a new continuous variable  $W_{l,i,i',t}$  and to add four sets of linear constraints that correspond to the McCormick envelopes<sup>8</sup>



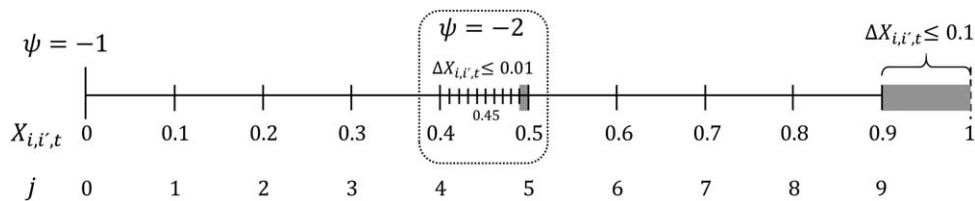


Figure 4. In multiparametric disaggregation, the continuous representation of variable  $X_{i,t}$  is achieved by discretizing the domain down to a certain level  $\psi$  and adding a bounded variable  $\Delta X_{i,t}$ .

$$W_{l,i,t} \geq x_{i,t}^L V_{l,i,t-1} + v_{l,i,t-1}^L X_{i,t} - v_{l,i,t-1}^L x_{i,t}^L \quad \forall i', i \in I_{i'} \cap B, l \in L_i, t > 1 \quad (18)$$

$$W_{l,i,t} \geq x_{i,t}^U V_{l,i,t-1} + v_{l,i,t-1}^U X_{i,t} - v_{l,i,t-1}^U x_{i,t}^U \quad \forall i', i \in I_{i'} \cap B, l \in L_i, t > 1 \quad (19)$$

$$W_{l,i,t} \leq x_{i,t}^L V_{l,i,t-1} + v_{l,i,t-1}^U X_{i,t} - v_{l,i,t-1}^U x_{i,t}^L \quad \forall i', i \in I_{i'} \cap B, l \in L_i, t > 1 \quad (20)$$

$$W_{l,i,t} \leq x_{i,t}^U V_{l,i,t-1} + v_{l,i,t-1}^L X_{i,t} - v_{l,i,t-1}^L x_{i,t}^U \quad \forall i', i \in I_{i'} \cap B, l \in L_i, t > 1 \quad (21)$$

In Eqs. 18–21, parameters  $x_{i,t}^L$ ,  $v_{l,i,t-1}^L$ ,  $x_{i,t}^U$ , and  $v_{l,i,t-1}^U$  are, respectively, the lower and upper bounds on variables  $X_{i,t}$  and  $V_{l,i,t-1}$ . Based on the domain of the split fraction variables, we can simply make  $x_{i,t}^L = 0$  and  $x_{i,t}^U = 1$ . The minimum amount of a liquid fuel in a tank is naturally zero:  $v_{l,i,t-1}^L = 0$ . For the upper bound, we can generate a time-dependent estimate. It is either the maximum capacity of the tank or the initial fuel amount plus incoming flows in such or preceding time intervals, see Eq. 22

$$v_{l,i,t}^U = \min \left[ v_{l,i,t}^{\max}, \sum_{i': l \in L_{i'}} \left( v_{l,i'}^0 + \sum_{t' \leq t} f_{l,i',t'}^{\text{in}} \right) \right] \quad \forall i, l \in L_i, t > 1 \quad (22)$$

It should be noted that the quality of the relaxation improves as the values of  $x_{i,t}^L$  and  $v_{l,i,t-1}^L$  increase and the values of  $x_{i,t}^U$  and  $v_{l,i,t-1}^U$  decrease. Tighter bounds can be generated using optimality-based bound tightening,<sup>42,43</sup> where each  $X_{i,t}$  and  $V_{l,i,t-1}$  variable is minimized and maximized over the constraints of the MILP relaxation.

### Bilinear terms in original formulation

The model with total flows and composition variables gives rise to two different sets of bilinear terms. As can be seen in the quality balances in Eq. 2, we have the product of compositions by total amounts  $C_{q,i,t} V_{i,t}$  as well as the product of compositions by total flows  $C_{q,i,t-1} F_{i,t}$ . Both bilinear terms have been relaxed in a similar manner using the following bounds:  $c_{q,i,t}^L = \min_{i': i' \notin D} c_{q,i'}^0$ ;  $c_{q,i,t}^U = \max_{i': i' \notin D} c_{q,i'}^0$ ;  $v_{l,i,t}^L = 0$ ;  $v_{l,i,t}^U = v_{l,i,t}^{\max}$ ;  $f_{i,t}^L = f_{i,t}^{\min}$ ;  $f_{i,t}^U = f_{i,t}^{\max}$ .

### MILP Relaxation with Multiparametric Disaggregation

A tighter formulation can be obtained using multiparametric disaggregation<sup>30,31</sup> that has been shown quite successful when dealing with scheduling problems involving blending in refineries<sup>4,13</sup> and hydroelectric power plants,<sup>43</sup> as well as with the steady-state design of water networks.<sup>36,38</sup> It works by discretizing one of the variables of each bilinear term down to a certain accuracy level  $\psi$ . While either set of variables  $X_{i,t}$  or

$V_{l,i,t}$  can be discretized, selecting the former makes it possible to give the same importance to all discretized variables using an overall value  $\psi \in \mathbb{Z}^-$ , as they already have a normalized  $[0, 1]$  domain. While there is no guarantee that this is the best option, it is the one chosen as it resulted in a better performance compared with commercial global optimization solvers for crude oil scheduling.<sup>4</sup> For the original formulation, the choice has been to discretize variables  $C_{q,i,t}$  because: (1) they are fewer than  $V_{i,t}$  and  $F_{i,t}$ ; (2) previous research for a water network problems<sup>36</sup> has shown that is preferable to discretize compositions over total flow rates.

Let  $k \in \{\psi, \psi+1, \dots, -1\}$  represent the set of powers of 10 over which split fraction variables  $X_{i,t}$  are discretized and let  $\Delta X_{i,t} \in [0, 10^\psi]$  be a new set of continuous variables that is added to obtain a continuous domain, see Figure 4 and Eq. 23. More specifically, new set of binary variables  $Z_{i,t,j,k}$  select the appropriate digit  $j$  for position  $k$ , ultimately leading to the value of  $X_{i,t}$  (together with  $\Delta X_{i,t}$ )

$$X_{i,t} = \sum_{k=\psi}^{-1} \sum_{j=1}^9 j \cdot 10^k \cdot Z_{i,t,j,k} + \Delta X_{i,t} \quad \forall i', i \in I_{i'} \cap B, t > 1 \quad (23)$$

The bilinear variables  $W_{l,i,t}$ , shared with the standard McCormick relaxation, are computed as a function of the two remaining sets of added nonnegative continuous variables,  $\hat{V}_{l,i,t,j,k}$  and  $\Delta W_{l,i,t}$  (Eq. 24). The former are disaggregated variables, related to the original amount variables  $V_{l,i,t-1}$  through Eq. 25. Equation 26 then ensures that they are different than zero only if the proper digit  $j$  has been selected for position  $k$ . Naturally, a single digit is activated for any given position, Eq. 27

$$W_{l,i,t} = \sum_{k=\psi}^{-1} \sum_{j=1}^9 j \cdot 10^k \cdot \hat{V}_{l,i,t,j,k} + \Delta W_{l,i,t} \quad \forall i', i \in I_{i'} \cap B, l \in L_i, t > 1 \quad (24)$$

$$V_{l,i,t-1} = \sum_{j=0}^9 \hat{V}_{l,i,t,j,k} \quad \forall i', i \in I_{i'} \cap B, l \in L_i, t > 1, k \in \{\psi, \dots, -1\} \quad (25)$$

$$v_{l,i,t-1}^L Z_{i,t,j,k} \leq \hat{V}_{l,i,t,j,k} \leq v_{l,i,t-1}^U Z_{i,t,j,k} \quad \forall i', i \in I_{i'} \cap B, l \in L_i, t > 1, k \in \{\psi, \dots, -1\}, j \in \{0, \dots, 9\} \quad (26)$$

$$\sum_{j=0}^9 Z_{i,t,j,k} = 1 \quad \forall i', i \in I_{i'} \cap B, t > 1, k \in \{\psi, \dots, -1\} \quad (27)$$

Variables  $\Delta W_{l,i,t}$  represent the bilinear term arising from  $V_{l,i,t-1} \Delta X_{i,t}$  in the derivation.<sup>31</sup> Due to the short domain of  $\Delta X_{i,t}$ , the bilinear term is relaxed using the McCormick envelopes, leading to Eqs. 28 and 29

**Table 1. Total Computational Time (CPUs), Upper Bounds (UB) from McCormick MILP Relaxation, and Subsequent Lower Bound (LB) from Constrained NLP for the Two Alternative Formulations (Global Optimal Solution in Bold)**

Formulation Problem	Total Flows and Compositions			Individual Flows and Split Fractions		
	TCPUs	LB (\$)	UB (\$)	UB (\$)	LB (\$)	TCPUs
029	0.45	<b>13,359.4</b>	13,359.4	13,359.4	<b>13,359.4</b>	0.58
146	0.89	Infeasible	46,917.0	45,896.5	Infeasible	1.33
480	1.25	Infeasible	9705.4	9443.2	8671.6	1.80
531	0.83	Infeasible	20,796.1	21,380.2	Infeasible	0.72
718	0.45	<b>7393.6</b>	7393.6	7393.6	<b>7393.6</b>	0.47
721	0.60	Infeasible	14,247.6	13,526.8	<b>13,526.8</b>	0.93
852	0.81	Infeasible	54,458.7	53,962.7	<b>53,962.7</b>	1.33

$$v_{l,i,t-1}^L \Delta X_{i,i',t} \leq \Delta W_{l,i,i',t} \leq v_{l,i,t-1}^U \Delta X_{i,i',t} \quad (28)$$

$$\forall i', i \in I_{i'} \cap B, l \in L_i, t > 1$$

$$10^\psi \left( V_{l,i,t-1} - v_{l,i,t-1}^U \right) + v_{l,i,t-1}^U \Delta X_{i,i',t} \leq \Delta W_{l,i,i',t} \quad (29)$$

$$\leq 10^\psi \left( V_{l,i,t-1} - v_{l,i,t-1}^L \right) + v_{l,i,t-1}^L \Delta X_{i,i',t}$$

$$\forall i', i \in I_{i'} \cap B, l \in L_i, t > 1$$

### MILP-NLP Algorithm for Global Optimization

Due to the nonconvex nature of the MINLP formulations, it may be difficult to find a feasible solution to the multiperiod pooling problem and even more to find the optimum and prove global optimality. A simple, yet systematic approach is to rely on the two-stage MILP-NLP solution procedure proposed by Jia et al.<sup>16</sup> The MILP model is generated by replacing every bilinear term with a new variable,<sup>16,20</sup> preferably adding the McCormick envelopes to generate a tighter relaxation.<sup>4,41</sup> Its solution provides the values of the binary variables to be fixed so as to generate a constrained version of the MINLP problem, now a NLP, which is solved in the second stage. The optimal value of the objective function in the MILP relaxation corresponds to an upper bound UB, whereas a feasible solution from the NLP provides a lower bound LB. The optimality gap is then computed as  $\text{Gap} = (\text{UB} - \text{LB}) / \text{UB}$ .

The issue with the McCormick relaxation is that it may be rather loose, potentially leading the two-stage procedure to failure. One way to increase the likelihood of getting a feasible

solution to the problem is to implement an outer-approximation algorithm<sup>44</sup> with integer cuts to exclude previous combinations of binary variables.<sup>41</sup> While this iterative procedure has the advantage of moving the UB toward the optimum, it is rather inefficient.

The chances of success considerably improve with a tighter relaxation. The piecewise McCormick envelopes<sup>9,29,45</sup> improve the quality of the relaxation by partitioning the domain of one of the variables in each bilinear term and have been used to tackle industrial problems dealing with crude oil scheduling<sup>46</sup> and synthesis of hydrogen networks.<sup>47</sup> In fact, by increasing the number of partitions, the relaxation can be as tight as desired. The multiparametric disaggregation technique described in the previous section achieves the same goal much more efficiently<sup>31</sup> with the resulting MILP becoming equivalent to the original MINLP as  $\psi \rightarrow -\infty$ . However, due to the increase in problem size, the MILP becomes increasingly more difficult to solve as  $\psi$  decreases, and so one should be cautious not to generate an intractable problem.<sup>33</sup>

The implemented global optimization algorithm is thus the following<sup>31,36</sup>: (1) Choose  $\psi = -1$ ; (2) Solve the MILP relaxation problem to obtain an upper bound UB and the values  $y_{i,i',t}$  of binary variables  $Y_{i,i',t}$ ; (3) Add constraint  $Y_{i,i',t} = y_{i,i',t}$  to the original MINLP reducing it to an NLP; (4) Using the solution from the MILP as a starting point, solve the NLP with a fast local solver to obtain the lower bound LB. If the NLP is infeasible, let  $\text{LB} = -\infty$ ; (5) If  $\frac{\text{UB} - \text{LB}}{\text{UB}} \leq \varepsilon$ , STOP, the solution is globally optimal within the given relative optimality tolerance  $\varepsilon$ . Otherwise, set  $\psi = \psi - 1$  and return to (2).

**Table 2. Key Computational Statistics for MILP-NLP Solution Strategy with Multiparametric Disaggregation (Global Optimal Solution in Bold, Maximum Computational Time in Italic, Gap Calculated with Respect to Global Optimal Solution, Which is not Necessarily the LB of the Corresponding Entry)**

Formulation Problem	$\psi$	Total Flows and Compositions				Individual Flows and Split Fractions			
		TCPUs	LB (\$)	UB (\$)	Gap (%)	Gap (%)	UB (\$)	LB (\$)	TCPUs
029	-1	0.71	<b>13,359.4</b>	13,359.4	0.0000	0.0000	13,359.4	<b>13,359.4</b>	0.76
146	-1	16.6	44,585.2	45,519.5	0.4898	0.1688	45,373.1	<b>45,296.6</b>	6.12
	-2	86.3	<b>45,296.6</b>	45,321.7	0.0555	0.0302	45,310.3	<b>45,296.6</b>	15.1
	-3	220	<b>45,296.6</b>	45,299.1	0.0056	0.0022	45,297.6	<b>45,296.6</b>	27.1
	-4	1899	<b>45,296.6</b>	45,296.9	0.0007	0.0003	45,296.7	<b>45,296.6</b>	81.3
	-5	<i>3600</i>	44,692.0	45,582.4	0.6270	0.0005	45,296.8	<b>45,296.6</b>	<i>3600</i>
480	-1	13.3	<b>9226.6</b>	9316.6	0.9657	0.0439	9230.7	9206.3	9.65
	-2	211	<b>9226.6</b>	9230.8	0.0452	0.0000	9226.6	<b>9226.6</b>	22.4
	-3	<i>3600</i>	9101.3	10,576.2	12.8				
531	-1	2.64	Inf.	20,458.9	2.05	0.0000	20,039.0	<b>20,039.0</b>	3.48
	-2	39	<b>20,039.0</b>	20,039.0	0.0000				
718	-1	0.85	<b>7393.6</b>	7393.6	0.0000	0.0000	7393.6	<b>7393.6</b>	0.77
721	-1	6.22	<b>13,526.8</b>	13,553.8	0.1992	0.0000	13,526.8	<b>13,526.8</b>	2.12
	-2	44.4	<b>13,526.8</b>	13,532.6	0.0430				
	-3	409	<b>13,526.8</b>	13,526.8	0.0000				
852	-1	3.00	<b>53,962.7</b>	53,962.7	0.0000	0.0000	53,962.7	<b>53,962.7</b>	4.36

**Table 3. Comparison Between New MILP-NLP Algorithm for Global Optimization and Commercial Global Optimization Solvers (CPUs for New Algorithm is the Minimum Between 3600 and the Sum Over  $\psi$  of the Individual Entries in Table 2)**

Problem	CPUs						Gap (%)					
	Total Flows and Compositions			Individual Flows and Split Fractions			Total Flows and Compositions			Individual Flows and Split Fractions		
	New	BARON	GloMIQO	New	BARON	GloMIQO	New	BARON	GloMIQO	New	BARON	GloMIQO
029	0.71	3.13	0.23	0.76	0.33	0.23		0.0001			0.0001	
146	3600	1227	3600	3600	91.3	488	0.0007	0.0001	0.7436	0.0003	0.0001	0.0001
480	3600	302	3600	32.0	453	3363	0.0452	0.0001	0.1386		0.0001	
531	41.6	97.4	3600	3.48	43.3	252	0.0001	0.0001	0.0332		0.0001	
718	0.85	3.56	0.22	0.77	3.97	0.32		0.0001			0.0001	
721	460	265	243	2.12	21.4	1.82		0.0001			0.0001	
852	3.00	231	600	4.36	134	3.91		0.0001			0.0001	

It should be noted that in theory, the worst-case scenario involves an infinite number of iterations to prove global optimality, but in practice, a few iterations are typically enough for the upper and lower bounds to converge or for the relaxation problem to become too complex to solve.

### Computational Results

The performance of the new MINLP formulation for the multiperiod pooling problem is now compared with the original one using the seven test problems from Kolodziej et al.<sup>13</sup> These feature six to eight tanks, three to four time periods, two qualities and can be identified by a three digit number. Note that the problem data and the GAMS model files corresponding to the original formulation and MILP-NLP global optimization algorithm are freely available in the MINLP library at [www.minlp.org](http://www.minlp.org), under the name multiperiod blend scheduling problem. The results reported next are, however, from a slightly improved formulation with fewer big-M constraints (recall the discussion of Eq. 5) and tighter bounds for the composition variables (as previously detailed), which has also benefited the performance of the commercial global optimization solvers.

The MINLP problems resulting from the two alternative formulations are tackled by: (1) the two-stage MILP-NLP algorithm relying on the McCormick relaxation; (2) the iterative MILP-NLP global optimization algorithm relying on the multiparametric disaggregation relaxation; and three commercial solvers: (3) DICOPT,<sup>48</sup> working on the wrong assumption that the relaxed nonlinear problem is convex and hence the most limiting; and global solvers: (4) BARON<sup>49</sup> 14.0 and (5) GloMIQO<sup>26</sup> 2.3.

All algorithms and mathematical formulations were implemented in GAMS 24.3 and solved on an Intel i7-4790 (3.6 GHz) processor with 8 GB of RAM, solid-state drive and running Windows 7, 64-bit operating system. CPLEX 12.6

running in parallel deterministic mode using up to eight threads has solved the MILP relaxation problems. The termination criterion was either a relative optimality tolerance equal to  $10^{-6}$  ( $\epsilon$ ) or a maximum computational effort of 3600 CPUs. Local optimization solver CONOPT<sup>50</sup> 3.16C tackled the NLP problems arising from the constrained MINLP (without the binary variables).

### Two-stage MILP-NLP solution approaches

We start the analysis by looking into the two-stage MILP-NLP solution strategy featuring the McCormick relaxation<sup>8</sup> of the bilinear terms. The results in Table 1 show that the main disadvantage of this approach is that a feasible solution cannot be guaranteed, which is more likely to occur for the formulation with total flows and compositions (5 vs. 2 failures). This is not totally surprising as the relaxation from the original formulation is of inferior quality (higher UB value) except for problem 531. Conversely, if a feasible solution can be found, we typically have  $LB = UB$ , meaning that it is proven globally optimal (the exception now comes from problem 480 when being solved by the new formulation, for which the LB of \$8671.6 is 6% below the global optimum of \$9226.6). The main advantage of the McCormick relaxation is that it originates MILPs that, like the subsequent NLPs, can be solved rather fast, leading to total computational times under two CPUs.

The very low computational time is an indication that the MILP can remain tractable with additional binary variables and constraints. It is thus worth to try tighter relaxation approaches like multiparametric disaggregation.<sup>30,31</sup> In Table 2, we give the results for the individual iterations of the global optimization algorithm described earlier. Again, the new formulation with individual flows and split fractions leads to the best results, with the two-stage solution approach being capable of proving optimality in under a minute for all but one

**Table 4. Statistics Related to Problem Size for MINLP Problems and Results for DICOPT Solver**

Problem	Binary Variables	Total Flows and Compositions					Individual Flows and Split Fractions				
		Total Variables	Equations	Bilinear Terms	CPUs	LB (\$)	LB (\$)	CPUs	Total Variables	Equations	Bilinear Terms
029	36	103	202	64	3.1	Inf.	Inf.	3.13	219	294	64
146	87	223	617	256	5.1	Inf.	43,325.7	2.41	689	965	480
480	124	313	879	376	8.86	Inf.	Inf.	8.7	941	1383	720
531	104	273	732	358	5.91	Inf.	Inf.	9.24	878	1218	684
718	87	223	603	244	1.15	5625.6	<b>7393.6</b>	1.15	672	939	456
721	87	223	623	256	5.21	Inf.	13,495.6	0.63	689	971	480
852	120	305	859	376	10.3	Inf.	<b>53,962.7</b>	1.71	933	1363	720

**Table 5. Results After Replacing the Constraint of Each Individual Stream to a Demand Tank Being Within its Composition Bounds with a More Realistic One (Individual Flows and Split Fraction Variables Model)**

Problem	Optimum (\$)	Improvement (%)	CPUs		
			New Algorithm	BARON	GloMIQO
029	13,359.4	0	0.57	0.33	0.29
146	47,889.2	5.72	468	72.6	159
480	13,062.6	41.6	2.68	94.7	2.75
531	22,481.8	12.2	2.69	75.1	1.43
718	7393.6	0	0.62	4.30	0.48
721	16,105.6	19.1	1.35	28.7	0.65
852	55,285.1	2.45	50.3	1002	368

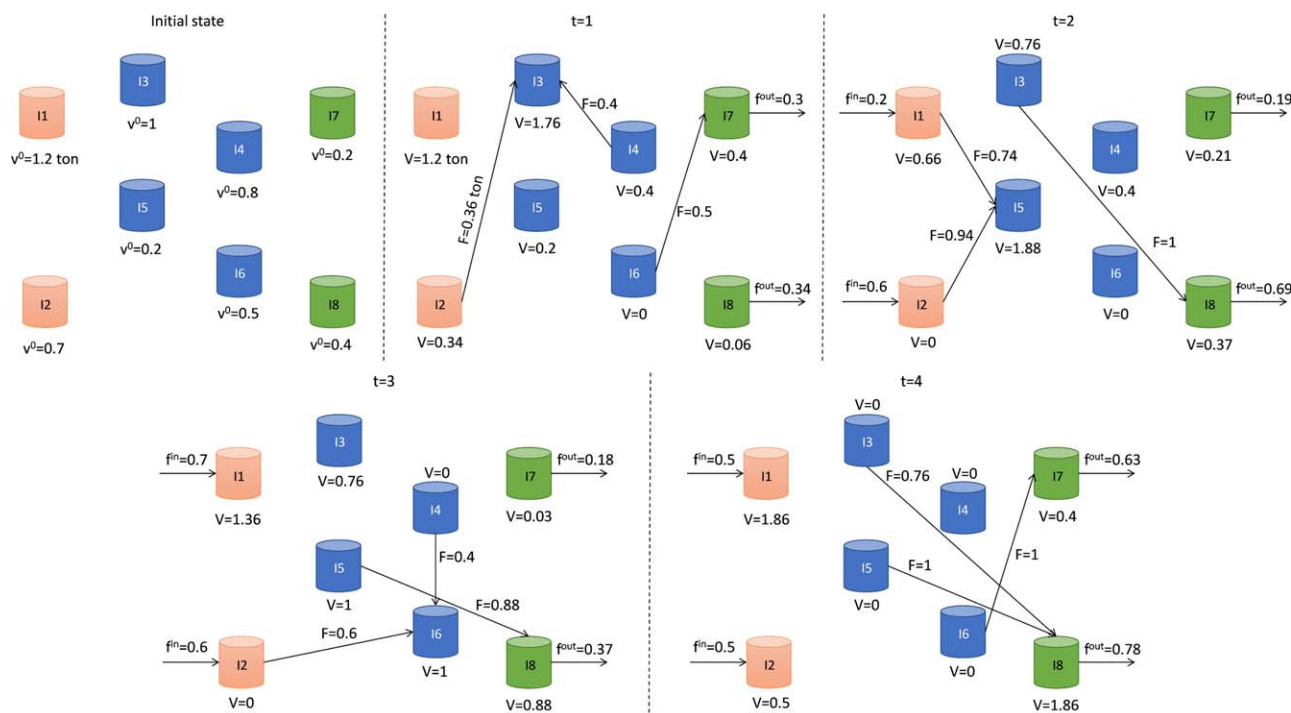
problem. For problem 146, a very low optimality gap of 0.0003% can be obtained for  $\psi = -4$  in 81.3 CPUs, which cannot be reduced for  $\psi = -5$  up to 1 h. In contrast, the original formulation leads to gaps equal to 0.0007% and 0.0452% for problems 146 and 480. Furthermore, it fails for problem 531 at  $\psi = -1$  and returns suboptimal solutions for problems 146 ( $\psi = -1, -5$ ) and 480 ( $\psi = -3$ ), compared with the single suboptimal solution of the new formulation for 480 ( $\psi = -1$ ). Overall, the two-stage MILP-NLP solution approach featuring multiparametric disaggregation in the relaxation stage is a much more efficient approach for the multiperiod pooling problem than the one based on the McCormick envelopes.

It should be mentioned at this point that Kolodziej et al.<sup>13</sup> report a zero optimality gap when solving the original formulation with multiparametric disaggregation. This is, however, due to the use of a higher relative optimality tolerance ( $10^{-3}$ ) coupled with the computation of the UB as the solution from the MILP instead of the best possible solution at the time of termination (check model files available online), which in this case can be up to 0.1% higher. As  $\psi$  decreases, closing the gap

from  $10^{-3}$  to  $10^{-6}$  becomes increasingly more difficult requiring considerably more computational resources than those reported.

### Commercial global solvers

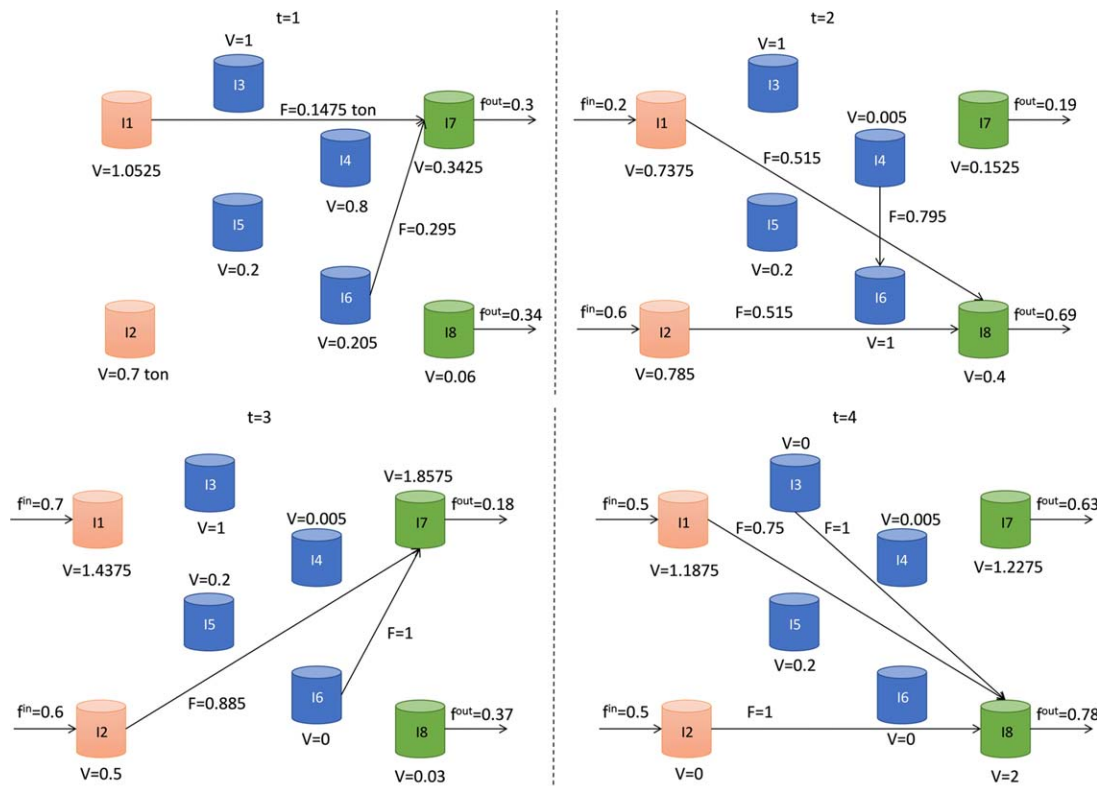
Table 3 provides the comparison between the proposed MILP-NLP iterative algorithm for global optimization relying on multiparametric disaggregation and the global solvers BARON and GloMIQO. The most notable result is that BARON is capable of solving all seven problems to global optimality regardless of the mathematical formulation being used, making it the best overall performer. This is a major improvement of version 14.0 over 10.2, which led to gaps as high as 134% for problem 480 after 2 h of computational time.<sup>13</sup> GloMIQO 2.3 is also much better than version 1.0, being capable of proving global optimality in four problems when using the formulation with total flows and compositions (compared with just one in Kolodziej et al.<sup>13</sup>). GloMIQO can also solve the MINLPs resulting from the new formulation in less than 1 h.



**Figure 5. Optimal operational plan for problem 480 and composition constraints to demand tanks enforced on every input stream (\$9226.6).**

[Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]





**Figure 6. Optimal operational plan for problem 480 and composition constraints to demand tanks enforced on input mixture (\$13062.6).**

[Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]

The results are more balanced in terms of computational time, with GloMIQO prevailing in the 2 + 4 problems for which the upper bound from the McCormick relaxation is the global optimal solution (recall the results in Table 1). For the remaining problems, the proposed algorithm is better if it is not needed to go deep into accuracy levels (low values of  $\psi$ ), which is the case of problems 531 and 852 (original formulation) and 480 and 531 (new formulation), the latter being solved one and two orders of magnitude faster compared with BARON and GloMIQO. The additional advantage of the proposed algorithm is that it can typically find a very good solution (often the global optimum) in a few seconds for  $\psi = -1$  (see Table 2), whereas BARON may take a few minutes to report the first feasible solution. In fact, if the former is provided as an initial point to BARON, the computational time is reduced by a factor of four or more.

#### Statistics related to problem size

The complexity of the MINLP formulations is better reflected on the poor performance of commercial solver DICOPT that iterates between NLP and MILP problems while assuming that the NLPs are convex. The results in Table 4 clearly show that this solver is not appropriate for this class of problems. Besides being unable to compute an optimality gap, it fails to find a feasible solution in six out of seven problems for the original formulation and returns a highly suboptimal solution for the other. Performance improves for the new formulation but it is still worse than the one obtained for the MILP-NLP strategy using the McCormick envelopes.

Table 4 also shows the statistics related to problem size, where the main observation is that the new formulation uses more continuous variables and constraints (the number of binary

variables is the same as the single set  $Y_{i,i',t}$  is shared by the two formulations) and leads to a larger number of bilinear terms.

#### Relaxing the constraint of all input streams to a demand tank being within its composition bounds

In the remarks of the problem statement section, it was mentioned that the assumption of all input streams to a demand tank being within its composition bounds is too restricting and may lead to suboptimal solutions. The real constraint is for the mix from all input streams to the tank to be within the bounds. It is translated into Eq. 30, which replaces Eqs. 5 and 15 in the individual flows and split fractions model

$$\begin{aligned}
 c_{q,i}^{\min} \sum_{i' \in I_i} \sum_{l \in L_{i'}} F_{l,i',i,t} &\leq \sum_{i' \in I_i} \sum_{l \in L_{i'}} c_{q,i} F_{l,i',i,t} \\
 &\leq c_{q,i}^{\max} \sum_{i' \in I_i} \sum_{l \in L_{i'}} F_{l,i',i,t} \quad \forall q, i \\
 &\in D, t
 \end{aligned}
 \tag{30}$$

Two aspects are worth emphasizing. The first is that the resulting model no longer features big-M constraints. The second is that the equivalent constraint in the total flows and composition variables model would be nonlinear as while the liquid compositions are known parameters, the feeding tanks compositions are variables. It reflects another disadvantage of the original formulation and is probably the reason why the constraints were proposed in the first place.

The results in Table 5 show that major improvements in solution quality can be obtained for problems 480 (41.6%), 721 (19.1%), and 531 (12.2%), whereas no benefits occur for problems 029 and 718. The new algorithm can now solve all problems to global optimality, with GloMIQO becoming the

best overall performer, benefiting from the fact that problems 146 and 852 are now the only ones for which the McCormick relaxation differs from the optimal solution.

### Optimal solution for problem 480

We end the discussion by presenting the optimal solutions considering the artificial and realistic composition constraints of inlet streams to a demand tank. Problem 480 is chosen for illustration because it is the one leading to the largest improvement. It features two supply, four blending and two demand tanks, and a total of  $|T| = 4$  time periods.

The optimal solution for the more restrictive case is worth \$9226.6 and is shown in Figure 5. Incoming flows to supply tanks occur at  $t \geq 2$  and there is demand for the two different products in all periods. Notice that the optimization takes full advantage of the operational flexibility of the network, activating different connections from one period to the next. It is thus worth to consider the multiperiod pooling problem over its steady-state counterpart. All blending tanks are useful and become empty at the end. It can be confirmed that they either send or receive fuel on a particular time slot. Still, there are multiple input streams for tanks I3, I5, I6, and I8 during  $t = 1, 2, 3$ , and 4, respectively.

In Figure 5, supply tanks I1 and I2 never send fuel to demand tanks I7 and I8 due to inadequate compositions. More specifically, the compositions of I1 (0.1; 0.2) (mass%) are below the minimum allowed compositions in both I7 (0.7; 0.3) and I8 (0.5; 0.3), whereas the compositions of I2 (0.9; 0.8) are above the maximum allowed compositions for quality one in I8 (0.8) and quality two in I7 (0.6). Replacing the composition constraint of the individual streams by the input mix makes it possible for the supply tanks to actively feed the demand tanks, provided that they are not alone. In fact, in the optimal solution given in Figure 6, worth \$13062.6 (41.6% higher), supply tanks I1 and I2 feed exclusively the demand tanks, completely bypassing the blending tanks. Notice for  $t = 1$  that mixing 147.5 kg of the liquid fuel in I1 with 295 kg of I6 at (1.0; 0.6) (mass%), leads to a blend with a (0.7; 0.467) composition, which is within the bounds of the destination demand tank I7.

### Conclusions

This article has presented a new MINLP formulation for the multiperiod pooling problem. Rather than considering total flows and composition variables to keep track of the properties of the tank mixtures throughout the planning periods, each blend initially present in a tank or due for entering the system is treated individually as a liquid fuel. This leads to a different set of complicating constraints with split fraction variables ensuring that the proportions of fuels exiting a tank are the same as the ones inside. While the new formulation is larger in size compared with the original, tighter relaxations of the nonconvex bilinear terms can generally be obtained, which is critical for finding high-quality solutions and ultimately proving global optimality.

Three commercial solvers and two MILP-NLP solution algorithms have been used to solve the MINLPs resulting from the alternative formulations, with the results showing improved performance for all five solution approaches. In particular, both BARON and GloMIQO can now solve the full set of literature test problems to global optimality. The practical implication of having a better formulation is that larger instances featuring more tanks, qualities and planning periods will still be tractable, potentially leading to more profitable operation of petroleum refineries.

### Acknowledgment

Financial support from Fundação para a Ciência e Tecnologia (FCT) through the Investigador FCT 2013 program.

### Notation

#### Sets/indices

$B$  = blending tanks  
 $D$  = demand tanks  
 $L/l$  = liquid fuel  
 $L_i$  = liquid fuels that can appear in tank  $i$   
 $I/i, i'$  = tanks  
 $I_p$  = tanks that can feed tank  $i'$   
 $j$  = digit in decimal numerical representation system,  $\in \{0, \dots, 9\}$   
 $k$  = position in decimal numerical representation system,  $\in \{\psi, \dots, -1\}$   
 $S$  = supply tanks  
 $T/t$  = planning time periods  
 $Q/q$  = qualities of mixture inside a tank

#### Parameters

$c_{q,l}$  = composition of quality  $q$  for liquid fuel  $l$ , mass%  
 $c_{q,i}^0$  = initial composition of quality  $q$  in tank  $i$ , mass%  
 $c_{q,i,t}^L$  = lower bound of variables  $C_{q,i,t}$   
 $c_{q,i,t}^U$  = upper bound of variables  $C_{q,i,t}$   
 $c_{q,i}^{\min}$  = minimum composition of quality  $q$  in tank  $i$ , mass%  
 $c_{q,i}^{\max}$  = maximum composition of quality  $q$  in tank  $i$ , mass%  
 $c_{i,i'}^x$  = fixed transfer cost between tanks  $i$  and  $i'$ , \$  
 $cs_{i,i'}^x$  = variable transfer cost between tanks  $i$  and  $i'$ , \$/kg  
 $f_{i,t}^{\text{in}}$  = mass arriving to supply tank  $i$  during time interval  $t$ , kg  
 $f_{l,i,t}^{\text{in}}$  = mass of liquid  $l$  arriving to supply tank  $i$  during time interval  $t$ , kg  
 $f_{i,i',t}^L$  = lower bound of variables  $F_{i,i',t}$   
 $f_{i,i'}^{\min}$  = minimum transfer mass between tanks  $i$  and  $i'$ , kg  
 $f_{i,i'}^{\max}$  = maximum transfer mass between tanks  $i$  and  $i'$ , kg  
 $f_{i,t}^{\text{out}}$  = mass removed from demand tank  $i$  during time interval  $t$ , kg  
 $f_{i,i',t}^U$  = upper bound of variables  $F_{i,i',t}$   
Gap = relative optimality gap, %  
LB = lower bound on value of objective function, \$  
 $p_i$  = value of transferring material from supply/to demand tank  $i$ , \$/kg  
UB = upper bound on value of objective function, \$  
 $v_i^0$  = initial inventory in tank  $i$ , kg  
 $v_{i,l}^0$  = initial inventory of liquid  $l$  in tank  $i$ , kg  
 $v_{i,t}^L$  = lower bound of variables  $V_{i,t}$   
 $v_{l,i,t}^L$  = lower bound of variables  $V_{l,i,t}$   
 $v_i^{\max}$  = maximum capacity of tank  $i$ , kg  
 $v_{i,t}^U$  = upper bound of variables  $V_{i,t}$   
 $v_{l,i,t}^U$  = upper bound of variables  $V_{l,i,t}$   
 $x_{i,i',t}^L$  = lower bound of variables  $X_{i,i',t}$   
 $x_{i,i',t}^U$  = upper bound of variables  $X_{i,i',t}$   
 $y_{i,i',t}$  = value of binary variables  $Y_{i,i',t}$  from MILP relaxation problem  
 $\varepsilon$  = target relative optimality tolerance  
 $\psi$  = accuracy level of discretized variables  $X_{i,i',t}$ ,  $\in \mathbb{Z}^-$

#### Variables

$Y_{i,i',t}$  = binary variable indicating mass flow between tanks  $i$  and  $i'$  during slot  $t$   
 $Z_{i,i',t,j,k}$  = binary variable assigning to discrete representation of  $X_{i,i',t}$  digit  $j$  to position  $k$   
 $C_{q,i,t}$  = composition of quality  $q$  in tank  $i$  at the end of slot  $t$ , mass%  
 $F_{l,i,i',t}$  = mass of liquid  $l$  transferred between tanks  $i$  and  $i'$  during slot  $t$ , kg  
 $F_{i,i',t}$  = total mass transferred between tanks  $i$  and  $i'$  during slot  $t$ , kg  
 $F_{l,i,t}^{\text{out}}$  = mass of liquid  $l$  removed from demand tank  $i$  during time interval  $t$ , kg  
 $V_{i,t}$  = total mass inside tank  $i$  at the end of slot  $t$ , kg  
 $V_{l,i,t}$  = mass of liquid  $l$  inside tank  $i$  at the end of  $t$ , kg  
 $\hat{V}_{l,i,i',t,j,k}$  = disaggregated variable from linearization of  $V_{l,i,t-1} Z_{i,i',t,j,k}$ , kg  
 $X_{i,i',t}$  = fraction of the contents of tank  $i$  leaving for  $i'$  during slot  $t$ ,  $\in [0, 1]$

$W_{i,j,t}$  = variable replacing bilinear term  $X_{i,j,t}V_{i,t-1}$ , kg  
 $\Delta X_{i,j,t}$  = slack variables for obtaining continuous domain of  $X_{i,j,t}$ ,  
 $\in [0, 10^6]$   
 $\Delta W_{i,j,t}$  = variable replacing bilinear term  $\Delta X_{i,j,t}V_{i,t-1}$ , kg

## Literature Cited

- Haverly CA. Studies of the behavior of recursion for the pooling problem. *SIGMAP Bulletin*. 1978;25:19–28.
- Quesada I, Grossmann IE. Global optimization of bilinear process networks with multicomponent flows. *Comput Chem Eng*. 1995;19:1219–1242.
- Galan B, Grossmann IE. Optimal design of distributed wastewater treatment networks. *Ind Eng Chem Res*. 1998;37:4036–4048.
- Castro PM, Grossmann IE. Global optimal scheduling of crude oil blending operations with RTN continuous-time and multiparametric disaggregation. *Ind Eng Chem Res*. 2014;53:15127–15145.
- Ben-Tal A, Eiger G, Gershovitz V. Global minimization by reducing the duality gap. *Math Program*. 1994;63:193–212.
- Tawarmalani M, Sahinidis NV. *Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming: Theory, Algorithms, Software, and Applications*. Dordrecht: Kluwer Academic Publishers, 2002:254–284.
- Alfaki M, Haugland D. Strong formulations for the pooling problem. *J Glob Optim*. 2013;56:897–916.
- McCormick GP. Computability of global solutions to factorable non-convex programs. Part I. Convex underestimating problems. *Math Program*. 1976;10:147–175.
- Meyer CA, Floudas CA. Global optimization of a combinatorially complex generalized pooling problem. *AIChE J*. 2006;52(3):1027–1037.
- Misener R, Gounaris CE, Floudas CA. Mathematical modeling and global optimization of large-scale extended pooling problems with the (EPA) complex emissions constraints. *Comput Chem Eng*. 2010;34:1432–1456.
- Furman KC, Androulakis IP. A novel MINLP-based representation of the original complex model for predicting gasoline emissions. *Comput Chem Eng*. 2008;32:2857–2876.
- Misener R, Floudas CA. Advances for the pooling problem: modeling, global optimization, and computational studies. *Appl Comput Math*. 2009;8(1):3–22.
- Kolodziej SP, Grossmann IE, Furman KC, Sawaya NW. A discretization-based approach for the optimization of the multiperiod blend scheduling problem. *Comput Chem Eng*. 2013;53:122–142.
- Kelly JD, Mann JL. Crude oil blend scheduling optimization: an application with multimillion dollar benefits-Part 1. *Hydrocarbon Process*. 2003;82(6):47–53.
- Lee H, Pinto JM, Grossmann IE, Park S. Mixed-integer linear programming model for refinery short-term scheduling of crude oil unloading with inventory management. *Ind Eng Chem Res*. 1996;35:1630–1641.
- Jia Z, Ierapetritou M, Kelly JD. Refinery short-term scheduling using continuous time formulation: crude-oil operations. *Ind Eng Chem Res*. 2003;42:3085–3097.
- Reddy PCP, Karimi IA, Srinivasan R. A new continuous-time formulation for scheduling crude oil operations. *Chem Eng Sci*. 2004;59:1325–1341.
- Furman K, Jia Z, Ierapetritou MG. A robust event-based continuous time formulation for tank transfer scheduling. *Ind Eng Chem Res*. 2007;46:9126–9136.
- Li J, Li W, Karimi IA, Srinivasan R. Improving the robustness and efficiency of crude scheduling algorithms. *AIChE J*. 2007;53:2659–2680.
- Mouret S, Grossmann IE, Pestiaux P. A novel priority-slot based continuous-time formulation for crude-oil scheduling problems. *Ind Eng Chem Res*. 2009;48:8515–8528.
- Yadav S, Shaik MA. Short-term scheduling of refinery crude oil operations. *Ind Eng Chem Res*. 2012;51:9287–9299.
- Hamisu AA, Kabantiok S, Wang M. Refinery scheduling of crude oil unloading with tank inventory management. *Comput Chem Eng*. 2013;55:134–147.
- Pantelides CC. Unified frameworks for the optimal process planning and scheduling. In: *Proceedings of the Second Conference on Foundations of Computer Aided Operations*. New York: Cache Publications, 1994:253.
- Castro PM, Barbosa-Póvoa AP, Matos HA, Novais AQ. Simple continuous-time formulation for short-term scheduling of batch and continuous processes. *Ind Eng Chem Res*. 2004;43:105–118.
- Sahinidis N. BARON: a general purpose global optimization software package. *J Glob Optim*. 1996;8:201–205.
- Misener R, Floudas CA. GloMIQO: global mixed-integer quadratic optimizer. *J. Glob Optim*. 2013;57:3–50.
- Misener R, Floudas CA. ANTIGONE: algorithms for coNTinuous/integer global optimization of nonlinear equations. *J Glob Optim*. 2014;59:503–526.
- Bergamini ML, Aguirre P, Grossmann IE. Logic-based outer approximation for globally optimal synthesis of process networks. *Comput Chem Eng*. 2005;29:1914–1933.
- Karupiah R, Grossmann IE. Global optimization for the synthesis of integrated water systems in chemical processes. *Comput Chem Eng*. 2006;30:650–673.
- Teles JP, Castro PM, Matos HA. Multiparametric disaggregation technique for global optimization of polynomial programming problems. *J Glob Optim*. 2013;55:227–251.
- Kolodziej S, Castro PM, Grossmann IE. Global optimization of bilinear programs with a multiparametric disaggregation technique. *J Glob Optim*. 2013;57:1039–1063.
- Wicaksono DN, Karimi IA. Piecewise MILP under- and overestimators for global optimization of bilinear programs. *AIChE J*. 2008;54:991–1008.
- Gounaris CE, Misener R, Floudas CA. Computational comparison of piecewise-linear relaxations for pooling problems. *Ind Eng Chem Res*. 2009;48:5742–5766.
- Hasan MMF, Karimi IA. Piecewise linear relaxation of bilinear programs using bivariate partitioning. *AIChE J*. 2010;56:1880–1893.
- Misener R, Thompson JP, Floudas CA. APOGEE: global optimization of standard, generalized, and extended pooling problems via linear and logarithmic partitioning schemes. *Comput Chem Eng*. 2011;35:876–892.
- Castro PM, Teles JP. Comparison of global optimization algorithms for the design of water-using networks. *Comput Chem Eng*. 2013;52:249–61.
- Faria DC, Bagajewicz MJ. A new approach for global optimization of a class of MINLP problems with applications to water management and pooling problems. *AIChE J*. 2012;58(8):2320–2335.
- Teles JP, Castro PM, Matos HA. Global optimization of water networks design using multiparametric disaggregation. *Comput Chem Eng*. 2012;40:132–47.
- Rubio-Castro E, Ponce-Ortega JM, Serna-González M, El-Halwagi MM, Pham V. Global optimization in property-based inter-plant water integration. *AIChE J*. 2013;59(3):813–33.
- Harjunkoski I, Maravelias C, Bongers P, Castro PM, Engell S, Grossmann I, Hooker J, Méndez C, Sand G, Wassick J. Scope for industrial applications of production scheduling models and solution methods. *Comput Chem Eng*. 2014;62:161–193.
- Karupiah R, Furman KC, Grossmann IE. Global optimization for scheduling refinery crude oil operations. *Comput Chem Eng*. 2008;32:2745–2766.
- Shectman JP, Sahinidis NV. A finite algorithm for global minimization of separable concave programs. *J Glob Optim*. 1998;12:1–35.
- Castro PM, Grossmann IE. Optimality-based bound contraction with multiparametric disaggregation for the global optimization of mixed-integer bilinear problems. *J Glob Optim*. 2014;59:277–306.
- Duran MA, Grossmann IE. An outer-approximation algorithm for a class of mixed-integer nonlinear programs. *Math Program*. 1986;36:307–339.
- Castro PM. Tightening piecewise McCormick relaxations for bilinear problems. *Comput Chem Eng*. 2015;72:300–311.
- Li J, Misener R, Floudas CA. Continuous-time modeling and global optimization approach for scheduling of crude oil operations. *AIChE J*. 2012;58:205–226.
- Jagannath A, Almansoori A. Modeling of hydrogen networks in a refinery using a stochastic programming Approach. *Ind Eng Chem Res*. 2014;53:19715–19735.
- Kocis GR, Grossmann IE. Computational experience with DICOPT solving MINLP problems in process systems engineering. *Comput Chem Eng*. 1989;13:307–315.
- Tawarmalani M, Sahinidis NV. A polyhedral branch-and-cut approach to global optimization. *Math Program*. 2005;103(2):225–249.
- Drud AS. CONOPT—a large-scale GRG code. *INFORMS J Comput*. 1994;6(2):207–216.

Manuscript received May 1, 2015, and revision received July 16, 2015.