New Multi-Commodity Flow Formulations for the Generalized Pooling Problem *

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Abstract: The generalized pooling problem is involved in many planning and scheduling problems in the petrochemical industry. Compared to the standard pooling problem where the blenders (or pools) are not allowed to be connected to one another, the generalized pooling problem has a more complex network structure and allows more types of problem formulations. The state-of-the-art generalized pooling formulations adopt a multi-commodity flow (MCF) strategy that was first proposed by Alfaki and Haugland (2013a) and proved to be stronger than the classical p-formulation. This paper proposes two new MCF formulations for the generalized pooling problem, using mixing and split fractions of blenders rather than the commodity flow fractions. The case study results show that, for some cases, the proposed formulations perform better than the existing MCF formulations, but none of the formulations dominates others for all cases. The results also show that formulations which have similar sizes and similarly tight linear programming relaxations may have dramatically different performance.

Keywords: Pooling problem; Multi-commodity flow; Global optimization; Blending; Network flow optimization.

1. INTRODUCTION

The pooling problem is a special type of network flow optimization problem, which was originally studied for gasoline blending in oil refineries (Haverly (1978)). In a pooling network, flows from different supply tanks are blended at blenders (or pools) and then sent to demand tanks to form final products. Since blending operation changes the flow qualities and it needs to be described with bilinear functions, the pooling problem is a nonconvex nonlinear programming (NLP) problem. The generalized pooling problem is an extension of the standard pooling problem where at least two blenders are connected to each other. The pooling problem has been recognized as an important class of optimization problems in the petrochemical industry (Bodington and Baker (1990)), because blending appears in many petrochemical processes.

Due to the nonconvexity of the pooling problem, the pooling problem is usually solved by a branch-and-bound based global optimization method, and the efficiency of the branch-and-bound search is known to be largely dependent on how tight the linear programming (LP) relaxation of the formulation is. Many pooling problem formulations have been studied in the literature (Gupte et al. (2017)). Well-known formulations for the standard pooling problem include P-, Q-, PQ-, and TP- formulations (Tawarmalani and Sahinidis (2002), Alfaki and Haugland (2013b)). The P-formulation models the blending operation using the flow rates and the flow qualities, while the Q-formulation replaces the flow qualities with the fractions of flows that come from the supply tanks. The PQ-formulation comprises the Q-formulation and extra strengthening constraints, and it is known to be stronger than the P- and Q-formulations. The TP-formulation is similar to the PQformulation but it uses the fractions of flows that go to the demand tanks. The TP-formulation sometimes performs better than the PQ-formulation and sometimes does not.

Recently, more attention has been paid to strong formulations of the generalized pooling problem. Alfaki and Haugland (2013a) proposed a multi-commodity flow (MCF) formulation, where the material in a supply tank is viewed as a monolithic commodity rather than a mixture of multiple components. They have shown that the MCF formulation reduces to the PQ-formulation for the standard pooling problem. Based on a similar idea, Boland et al. (2016) proposed a different MCF formulation that extends the TPformulation for the generalized pooling problem, where a commodity is defined to be the product in a demand tank. They also proposed some other MCF formulations that combine the supply commodities, demand commodities, and commodity paths in different ways, and in their extensive case studies the supply commodity and the demand commodity based formulations performed better than the other formulations. On the other hand, a rather different modeling strategy has been used in the field of process sys-

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tems engineering (e.g., Quesada and Grossmann (1995)). In this strategy, the blending operation is modeled with individual components in the flows and the blender split fractions. Based on this strategy, Lotero et al. (2016) proposed a multi-commodity based split fraction formulation for multi-period blending problem, and they proved that this formulation leads to tighter LP relaxations than the component based split fraction formulation. Note that the multi-period blending problem in their work differs from the generalized pooling problem considered in this paper, because it considers the fractions of tank inventories rather than the fractions of tank throughputs.

This paper is concerned with strong formulations for the generalized pooling problem. There are two major contributions of the paper. One contribution is the proposal of two new MCF formulations, where the first one is similar to the one proposed by Lotero et al. (2016) for multi-period blending, and the second one is a new formulation based on mixing fractions and demand commodities. The other contribution is to show through case studies that, the two new MCF formulations sometimes perform better than the MCF formulations in the literature, but no formulation is always better than the others. In addition, the formulations can have significantly different performance even when their sizes are similar and their LP relaxations (at root nodes) are similarly tight.

The remaining part of the paper is organized as follows: Section 2 provides a descriptive problem statement with a list of symbols. Section 3 introduces two representative MCF formulations in the literature. Section 4 proposes two new MCF formulations that use blender mixing and split fractions, respectively. Section 5 compares the performance of the four MCF formulations through three case study problems. The paper ends with concluding remarks in Section 6.

2. PROBLEM STATEMENT

The generalized pooling network can be viewed as a acyclic graph G = (N, A). The set of nodes N consists of three subsets S, B, D, which include supply tanks, blenders, and demand tanks, respectively. The set of arcs A includes all allowable connections between two tanks. In operation of the pooling network, material flows leave the supply tanks, and they are blended once or multiple times before entering the demand tanks. The goal of optimization is to determine the flow rates along all arcs of the network such that the total profit is maximized. Since the operation is assumed to be at a steady state, the inventory levels of the tanks are not considered in the problem. A general descriptive optimization formulation is given below:

- min. Negative profit
- s.t. (1) Flow quality change through blenders;
 - (2) Mass balance around blenders;
 - (3) Bounds on product qualities;
 - (4) Bounds on total flows going through tanks;
 - (5) Bounds on individual variables.

In the above formulation, constraint (1) restricts how flow qualities change through blending; constraint (2) enforces mass balance for the inlet flows and outlet flows of each blender; constraint (3) observes quality specifications of

Table 1. Notation for the pooling formulations

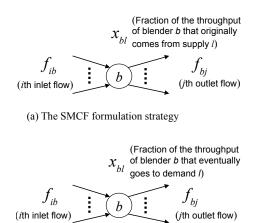
Sets						
S	Set of supply tanks					
B	Set of blenders					
D	Set of demand tanks					
N	Set of all tanks in the network					
A	Set of allowable arcs in the network					
K	Quality of interest					
S_i	Set of supply commodities in tank i					
D_i	Set of demand commodities in tank \boldsymbol{i}					
Parameters						
β_s	Unit cost of material in supply tank s					
β_d	Unit price of product in demand $tank d$					
$\lambda_{s,k}$	Quality k in supply tank s					
$\lambda_{d,k}^{U}$	Upper bound on quality k for demand tank d					
$\lambda_{d,k}^U$ μ_i^U	Upper bound on capacity of tank i					
Variables						
$f_{i,j}$	Flow rate along arc (i, j)					
$f_{i,j,l}/z_{i,j,l}$	Commodity flow l along arc (i, j)					
$z_{i,b,j,l}$	Commodity flow l along path (i, b, j)					
$x_{i,l}/x_{j,l}$	Commodity l fraction of throughput of tank i/j					
x_{ib}/x_{bj}	Mixing/split fraction at blender b					

products in the demand tanks (such as concentration of a key chemical component); constraint (4) represents bounds on total flow rates through each tank, which result from the availability of materials, the blending capacity, and the costumer demands; constraint (5) imposes bounds on individual variables, such as non-negativity bounds of flow rates. Table 1 shows a list of symbols are will be used for the mathematical formulations in the subsequent sections.

The existing generalized pooling formulations differ primarily in the way to model constraint (1) (and accordingly constraint (2) as well). The classical P-formulation explicitly includes flow qualities as variables, and the change of flow qualities can be described by bilinear equations involving flow qualities and flow rates. The MCF formulations use a different idea, where the flow qualities are not defined as variables explicitly. In these formulations, each physical flow is logically disaggregated into several parts, and each part is called a commodity flow that is defined to originally come from a supply tank or eventually go to a demand tank. The quality of a physical flow can be calculated from the composition of the flow (in terms of the commodities). It has been proven that the MCF formulations lead to tighter LP relaxations than the Pformulation and therefore favor branch-and-bound based global optimization (Alfaki and Haugland (2013a), Boland et al. (2016)).

3. TWO REPRESENTATIVE MCF FORMULATIONS FROM THE LITERATURE

This section introduces two representative MCF formulations, proposed by Alfaki and Haugland (2013a) and Boland et al. (2016) respectively. They are called supply based MCF formulation (SMCF) and demand based MCF formulation (DMCF) in this paper. According to the extensive simulations studies by Boland et al. (2016), SMCF and DMCF formulations usually outperform other MCF formulations in the literature.



(b) The DMCF formulation strategy

Fig. 1. Illustration of SMCF and DMCF strategies

3.1 The Supply Based MCF Formulation

In the SMCF formulation, a commodity flow l in a physical flow is the part of the flow that originally comes from supply tank $l \ (\in S)$, and it is called supply commodity flow in the paper for convenience. The ratio of the supply commodity flows to the physical flow are defined as fractional variables, and the composition of a physical flow can be calculated from the supply commodity fractions in that flow. Obviously, the supply commodity fractions in flow (i, j) equal to those in tank *i*. For a blender, the inlet flows may have different supply commodity fractions but the outlet flows must have the same fractions to each other. This strategy to model the flow composition change is illustrated by Figure 1(a). The mathematical SMCF formulations is shown below:

Objective:

$$\min \quad \sum_{(s,j)\in A} \beta_s f_{sj} - \sum_{(i,d)\in A} \beta_d f_{id}$$
(SMCF-1)

Supply commodity fraction:

$$z_{ijl} = f_{ij}x_{il}, \quad \forall (i,j) \in A, l \in S_i$$
 (SMCF-2)

$$\sum_{l \in S_b} x_{bl} = 1, \quad \forall b \in B \tag{SMCF-3}$$

Mass balance:

$$\sum_{(i,b)\in A} z_{ibl} = \sum_{(b,l)\in A} z_{bjl}, \quad \forall b \in B, l \in S_b \qquad (\text{SMCF-4})$$

Quality bounds:

$$\sum_{(i,d)\in A} \sum_{l\in S_i} z_{idl}\lambda_{sk} \le \sum_{(i,d)\in A} \sum_{l\in S_i} z_{idl}\lambda_{dk}^U, \quad \forall d\in D, k\in K$$
(SMCF-5)

Node capacity:

$$\sum_{(i,j)\in A} f_{ij} \le \mu_i^U, \quad \forall i \in N \backslash D$$
 (SMCF-6)

$$\sum_{(i,d)\in A} f_{id} \le \mu_d^U, \quad \forall d \in D$$
 (SMCF-7)

Variable bounds:

$$0 \le x_{bl} \le 1, \quad \forall b \in B, l \in S_b$$
 (SMCF-8)

$$f_{ij} \ge 0, \quad \forall (i,j) \in A$$
 (SMCF-9)

Strengthening constraints:

$$\sum_{l \in S_b} z_{bjl} = f_{bj}, \quad \forall b \in B, (b, j) \in A$$
 (SMCF-10)

$$\sum_{(b,j)\in A} z_{bjl} \le \mu_b^U x_{bl}, \quad \forall b \in B, l \in S_b$$
(SMCF-11)

In the SMCF formulation, x_{il} denotes the fraction for supply commodity l in tank i. The bilinear equation (SMCF-2) enforces the same x_{il} for the outlet flows of tank i. When i = s (i.e., i is a supply tank), x_{sl} is a parameter, which is 1 when l = s and 0 when $l \neq s$; in this case, (SMCF-2) reduces to a linear equation. If the problem contains only one supply tank (i.e., |S| = 1), then the problem reduces to a LP problem. The unity equation (SMCF-3) states the fact that any part of a flow through a blender must come from one of the supply tanks.

The strengthening constraints (SMCF-10) and (SMCF-11) are obtained via the reformulation-linearization technique (RLT) (Sherali and Alameddine (1992)). They are redundant for modeling the problem but can tighten the LP relaxation of the formulation for efficient global optimization. Specifically, (SMCF-10) comes from multiplying both sides of (SMCF-3) by f_{bj} , and (SMCF-11) from multiplying both sides of (SMCF-6) by x_{bl} .

3.2 The Demand Based MCF Formulation

While SMCF is an extension of the PQ-formulation for the generalized pooling problem, DMCF is an extension of the TP-formulation. In the DMCF formulation, a commodity flow l is defined to be the part of a flow that eventually goes to demand tank $l \ (\in D)$, and for convenience, it is called a demand commodity flow in this paper. Consequently, the ratio of the demand commodity flows to the physical flow are expressed as fractional variables. In contrast to the supply commodity fractions, the demand commodity fractions in flow (i, j) equal to those in tank j. For a blender, the inlet flows must have the same demand commodity fractions. This strategy is illustrated by Figure 1(b), and the DMCF formulation is shown below:

Objective:

min
$$\sum_{(s,j)\in A} \beta_s f_{sj} - \sum_{(i,d)\in A} \beta_d f_{id}$$
 (DMCF-1)

Demand commodity fraction:

$$z_{ijl} = f_{ij}x_{jl}, \quad \forall (i,j) \in A, l \in D_j$$
 (DMCF-2)

$$\sum_{l \in D_{t}} x_{bl} = 1, \quad \forall b \in B \tag{DMCF-3}$$

Mass balance:

$$\sum_{(i,b)\in A} z_{ibl} = \sum_{(b,j)\in A} z_{bjl}, \quad \forall b \in B, l \in D_b \quad \text{(DMCF-4)}$$

Quality bounds:

$$\sum_{s \in S} \sum_{(s,j) \in A} z_{sjl} \lambda_{sk} \le \sum_{s \in S} \sum_{(s,j) \in A} z_{sjl} \lambda_{lk}^{U}, \quad \forall l \in D, k \in K$$
(DMCF-5)

Node capacity:

$$\sum_{(i,j)\in A} f_{ij} \le \mu_j^U, \quad \forall i \in N \backslash D$$
 (DMCF-6)

$$\sum_{(i,d)\in A} f_{id} \le \mu_d^U, \quad \forall d \in D$$
 (DMCF-7)

Variable bounds:

$$0 \le x_{bl} \le 1, \quad \forall b \in B, l \in D_b$$
 (DMCF-8)
$$f_{ii} > 0, \quad \forall (i, j) \in A$$
 (DMCF-9)

Strengthening constraints:

$$\sum_{a \in D_i} z_{ibl} = f_{ib}, \quad \forall b \in B, (i, b) \in A$$
 (DMCF-10)

$$\sum_{(i,b)\in A} z_{ibl} \le \mu_b^U x_{bl}, \quad \forall b \in B, l \in D_b \qquad (\text{DMCF-11})$$

Here x_{il} stands for the fraction for demand commodity l in tank i. When i = d, x_{dl} is a parameter, which is 1 when l = d and 0 when $l \neq d$, and the bilinear equation (DMCF-2) reduces to a linear equation. The strengthening constraints are obtained by the RLT technique from constraints (DMCF-3) and (DMCF-6).

4. THE NEW MCF FORMULATIONS

The new MCF formulations are motivated by the multicomponent flow strategy that was originally proposed in the process systems engineering community (Quesada and Grossmann (1995)). The main idea of this strategy is to disaggregate a physical flow into flows of the involved chemical components. At a blender, all inlet chemical component flows are split to different outlets with the same split fractions. Lotero et al. (2016) proposed a similar strategy that disaggregate the physical flows into supply commodity flows rather than chemical component flows, and applied the strategy to multi-period blending (where the split fractions are fractions of tank inventories rather than the tank throughputs). In this section, the formulation by Lotero et al. (2016) is modified for the generalized pooling problem, and the resulting formulation is called the supply and split fraction (SSF) based formulation. After that, a new formulation is proposed based on the demand commodity flow and the mixing fractions at the blenders. This formulation is called demand and mixing fraction (DMF) based formulation.

4.1 The Supply and Split Fraction Based Formulation

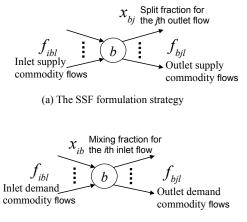
The SSF formulation involves the supply commodity flows along all arcs but not the physical flows (except for the supply tank outlet flows that contain only one commodity by definition). In order to model the flow composition change, the split fractions of the blenders x_{bj} are defined. This strategy is illustrated by Figure 2(a), and the SSF formulation is shown below:

Objective:

$$\min \quad \sum_{s \in S} \sum_{(s,j) \in A} \beta_s f_{sj} - \sum_{d \in D} \sum_{(i,d) \in A} \sum_{l \in S_d} \beta_d f_{idl} \quad (\text{SSF-1})$$

Blender split fraction:

$$z_{ibjl} = f_{ibl} x_{bj}, \quad \forall b \in B, (i, b), (b, j) \in A, l \in S_b \quad (\text{SSF-2})$$



(b) The DMF formulation strategy

Fig. 2. Illustration of SSF and DMF strategies

$$\sum_{(b,j)\in A} x_{bj} = 1, \quad \forall b \in B$$
 (SSF-3)

Mass balance:

$$f_{bjl} = \sum_{(i,b)\in A} z_{ibjl}, \quad \forall b \in B, (b,j) \in A, l \in S_b \quad (\text{SSF-4})$$

Quality bounds:

$$\sum_{(i,d)\in A} \sum_{l\in S_i} f_{idl}\lambda_{dk} \le \sum_{(i,d)\in A} \sum_{l\in S_i} f_{idl}\lambda_{dk}^U, \quad \forall d\in D, k\in K$$
(SSF-5)

Node capacity:

$$\sum_{(i,j)\in A} \sum_{l\in S_i} f_{ijl} \le \mu_i^U, \quad \forall i \in N \setminus D$$
 (SSF-6)

$$\sum_{(i,j)\in A} \sum_{l\in S_i} f_{idl} \le \mu_d^U, \quad \forall d \in D$$
 (SSF-7)

Variable bounds:

$$0 \le x_{bj} \le 1, \quad \forall b \in B, (b, j) \in A$$
 (SSF-8)

$$f_{ijl} \ge 0, \quad \forall (i,j) \in A, l \in S_i$$
 (SSF-9)

Strengthening constraints:

$$\sum_{(b,j)\in A} z_{ibjl} = f_{ibl}, \quad \forall b \in B, (i,b) \in A, l \in S_b \quad (\text{SSF-10})$$

$$\sum_{(i,b)\in A} \sum_{l\in S_i} z_{ibjl} \le \mu_b^U x_{bj}, \quad \forall b\in B, (b,j)\in A \quad (\text{SSF-11})$$

In the above formulation, the bilinear equation (SSF-2) enforces the same split fraction for all inlet commodity flows, and z_{ibjl} actually represents the rate of demand commodity l that comes from tank i to tank j through blender b. (SSF-2) states that the sum of the split fractions is one. The strengthening constraints are obtained from constraints (SSF-3), (SSF-6).

4.2 The Demand and Mixing Fraction Based Formulation

The DMF formulation uses the demand commodity flow rather than the supply commodity flow. Note that at a blender, the fraction of an inlet demand commodity flow that goes to an outlet does not equal to the blender split fraction. For example, the fraction of an inlet demand commodity flow l that goes to an outlet is 0 if the outlet is not on a path to demand tank l, no matter what the split fraction for the outlet is. On the other hand, the inlet demand commodity flows contribute to any outlet demand commodity flows with the same fractions, which equal to the mixing fractions of the inlets. For example, assume x_{ib} to be the fraction for the *i*th inlet flow in the total inlet flow. Then for any outlet demand commodity flow f_{bjl} (i.e., the part of outlet flow f_{bj} that eventually goes to demand tank l), x_{ib} of it comes from the *i*th inlet. This strategy is illustrated in Figure 2(b), and the DMF formulation is as follows:

Objective:

$$\min \sum_{s \in S} \sum_{(s,j) \in A} \sum_{l \in D_s} \beta_s f_{sjl} - \sum_{d \in D} \sum_{(i,d) \in A} \beta_d f_{id} \quad (\text{DMF-1})$$

Blender mixing fraction:

$$z_{ibjl} = f_{bjl} x_{ib}, \ \forall b \in B, (i, b), (b, j) \in A, l \in D_b \ (DMF-2)$$

$$\sum_{(i,b)\in A} x_{ib} = 1, \quad \forall b \in B$$
 (DMF-3)

Mass balance:

$$f_{ibl} = \sum_{(b,j)\in A} z_{ibjl}, \quad \forall b \in B, \forall (i,b) \in A, l \in D_b \text{ (DMF-4)}$$

Quality bounds:

$$\sum_{s \in S} \sum_{(s,j) \in A} f_{sjl} \lambda_{sk} \le \sum_{s \in S} \sum_{(s,j) \in A} f_{sjl} \lambda_{sk}^{U}, \quad \forall l \in D, k \in K$$
(DMF-5)

Node capacity:

$$\sum_{(i,j)\in A} \sum_{l\in D_j} f_{ijl} \le \mu_i^U, \quad \forall i \in N \setminus D$$
 (DMF-6)

$$\sum_{(i,d)\in A} \sum_{l\in D_d} f_{idl} \le \mu_d^U, \quad \forall d\in D$$
 (DMF-7)

Variable bounds:

$$0 \le x_{ib} \le 1, \quad \forall b \in B, (i,b) \in A \tag{DMF-8}$$

$$f_{ijl} \ge 0, \quad \forall (i,j) \in A, l \in D$$
 (DMF-9)

Strengthening constraints:

$$\sum_{(i,b)\in A} z_{ibjl} = f_{bjl}, \quad \forall b \in B, (b,j) \in A, l \in D_b \text{ (DMF-10)}$$

$$\sum_{(b,j)\in A} \sum_{l\in D_b} z_{ibjl} \le \mu_b^U x_{ib}, \quad \forall b\in B, (i,b)\in A \quad (\text{DMF-11})$$

The above strengthening constraints are obtained from constraints (DMF-3), (DMF-6). Note that the left-hand-side of quality constraint (DMF-5) represents the total quality k (contributed by demand commodities from all supply thanks) entering demand tank l, and the right-hand-side of the constraint represents the maximum quality k allowed to enter the same tank.

5. SIMULATION STUDIES

The purpose of the simulation study is to demonstrate that the four MCF formulations, especially the last three

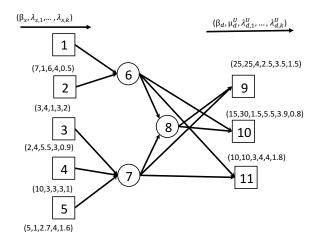
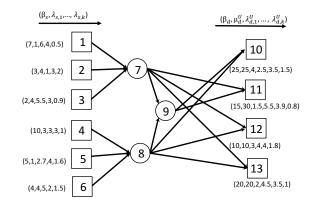
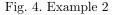


Fig. 3. Example 1





that have not attracted much attention form the process systems engineering community, have significant computational advantages for certain problem instances. Due to the page limit of the paper, only three examples are presented and discussed here. Examples 1 and 2 are depicted in Figures 3 and 4 respectively, where the values of parameters used are also labeled. Example 3 is adapted from a natural gas production network operation problem that was originally developed in Selot (2009). The basic problem information can be found in Li et al. (2011), but in addition to CO₂, five more components are considered, including N_2 , C_2 , C_3 , C_4 , C_{5+} . The quality constraints are the upper bounds of the six components, given in Table 4.1 in Selot (2009). In addition, gas price (i.e., β_d) is changed into 0.00536417 (\$/mol) and the gas costs (i.e., β_s) are also updated and shown in Table 2.

The case studies were performed on a virtual machine with a 3.40 GHz CPU, 4GB memory, and Ubuntu 16.02 operating system. The case study problems were formulated on GAMS 24.8.5 (Bussieck and Meeraus (2004)) and solved by BARON 17.4.1 Tawarmalani and Sahinidis (2005). For all cases, the relative termination tolerance is 10^{-3} .

Table 3 provides the topological information, number of qualities, and the optimal objective values of the example problems (where $|\cdot|$ denotes the cardinality of a set). The computational results with the four MCF formulations are shown in Table 4, from which we can have the following

Table 2. Cost (β_s) information for Example 3

Gas Field	D35	BY	\mathbf{SC}	E11	F6	F23SW
$\beta_s \ (\$/mol)$	0.001	0.001	0.001	0.003	0.001	0.002
Gas Field	F23	BN	B11	HL	SE	M3
$\beta_s \; (\text{mol})$	0.003	0.002	0.004	0.001	0.002	0.001
Gas Field	M4	M1	JN			
$\beta_s \ (\text{mol})$	0.001	0.002	0.001			

Table 3. Case study problem characteristics

	S	B	D	A	K	Obj
Ex. 1	5	3	3	13	4	-549.8
Ex. 2	6	3	4	16	4	-570.7
Ex. 3	15	13	3	34	6	-22.9924

Table 4. Results for the four MCF formulations

Cases	Formulations	Bilinear equ.			Time	Rel. gap at
		\mathbf{Z}	f	х	(s)	root node
Ex. 1	SMCF	25	8	10	24.2	55.67%
	DMCF	19	7	8	1.1	55.74%
	SSF	59	23	8	3.5	55.74%
	DMF	53	22	7	1.2	55.74%
Ex. 2	SMCF	48	10	15	4.7	96.73%
	DMCF	28	8	10	20.6	98.22%
	SSF	132	39	10	314.5	98.22%
	DMF	104	36	8	0.3	98.11%
Ex. 3	SMCF	79	14	58	31.8	4.46%
	DMCF	60	30	23	2.1	1.11%
	SSF	186	93	8	1.0	5.32%
	DMF	81	29	28	23.7	5.32%

interesting observations. First, none of the formulations dominates the others for all examples. Second, for certain example (i.e., Example 2), the solution times with different formulations can differ by three orders of magnitude. This indicates the importance of formulation selection for the generalized pooling problem, even when the formulations to be selected from are all believed to be stronger than the P-formulation. Third, the number of bilinear terms and/or the number of variables involved in the bilinear terms do not tell whether the formulation is favorable. For example, the two new MCF formulations have more bilinear terms for all the examples, but they do outperform the SMCF and DMCF formulations significantly for some of the examples. Finally, the tightness of the LP relaxation does not tell whether the formulation is favorable. In Examples 1 and 2, the four formulations have similar relative optimality gaps at the root node (in the branch-and-bound tree), but their performance can be dramatically different. In Example 3, the best formulation actually has the largest relative gap at the root node.

6. CONCLUDING REMARKS

According to the best of our knowledge, the DMCF, SSF, DMF formulations have not attracted much attention for the generalized pooling problem within the process systems engineering community. The case study results indicate that one may consider using these formulations when the classical P-formulation and the SMCF formulation do not work well. The case study results also show that, the LP relaxation and the problem size, which are widely accepted criteria to assess the generalized pooling formulation, are not the only factors determining the performance of the formulation. A rigorous theoretical explanation for our findings is an open question for the future research.

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