

# STRONG CONVEX NONLINEAR RELAXATIONS OF THE POOLING PROBLEM

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**Abstract.** We investigate new convex relaxations for the pooling problem, a classic nonconvex production planning problem in which input materials are mixed in intermediate pools, with the outputs of these pools further mixed to make output products meeting given attribute percentage requirements. Our relaxations are derived by considering a set which arises from the formulation by considering a single product, a single attribute, and a single pool. The convex hull of the resulting nonconvex set is not polyhedral. We derive valid linear and convex nonlinear inequalities for the convex hull, and demonstrate that different subsets of these inequalities define the convex hull of the nonconvex set in three cases determined by the parameters of the set. Computational results on literature instances and newly created larger test instances demonstrate that the inequalities can significantly strengthen the convex relaxation of the  $pq$ -formulation of the pooling problem, which is the relaxation known to have the strongest bound.

**1. Introduction.** The pooling problem is a classic nonconvex nonlinear problem introduced by Haverly in 1978 [21]. The problem consists in routing flow through a feed forward network from inputs through pools to output products. The material that is introduced at inputs has known quality for certain attributes. The task is to find a flow distribution that respects quality restrictions on the output products. As is standard in the pooling problem, we assume linear blending, i.e., the attributes at a node are mixed in the same proportion as the incoming flows. As the quality of the attributes in the pools is dependent on the decisions determining amount of flow from inputs to the pools, the resulting constraints include bilinear terms.

The aim of this work is to strengthen the relaxation of the strongest known formulation, i.e., the so-called  $pq$ -formulation proposed in [30, 34]. By focusing on a single output product, a single attribute, and a single pool, and aggregating variables, we derive a structured nonconvex 5-variable set that is a relaxation of the original feasible set. The description of this set contains one bilinear term which captures some of the nonconvex essence of the problem. Valid convex inequalities for this set directly translate to valid inequalities for the original pooling problem. We derive valid linear and nonlinear convex inequalities for the set. For three cases determined by the parameters of the set, we demonstrate that a subset of these inequalities define the convex hull of the set. Finally, we conduct an illustrative computational study that demonstrates that these inequalities can indeed improve the relaxation quality over the  $pq$ -formulation, particularly on instances in which the underlying network is sparse, which are precisely the instances in which the  $pq$ -formulation relaxation has the largest gap to the optimal value. As part of this study, we create and test the inequalities on new, larger test instances of the pooling problem.

The remainder of the paper is organized as follows. We briefly review relevant literature on the pooling problem in the remainder of this section. In [section 2](#), we introduce the  $pq$ -formulation, and its classic relaxation based on the McCormick relaxation. Our set of interest, that represents a relaxation of the pooling problem,

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is introduced in [section 3](#). In the same section, we present the valid inequalities for this set. We then prove in [section 4](#) that certain subsets of the proposed inequalities define the convex hull of the set of interest, for three cases based on the parameters of the set. Computational results are presented in [section 5](#), and concluding remarks are made in [section 6](#).

**1.1. Literature Review.** There are many applications of the pooling problem, including petroleum refining, wastewater treatment, and general chemical engineering process design [[5](#), [12](#), [23](#), [31](#)]. This is confirmed by an interesting analysis performed by Ceccon et al. [[10](#)] whose method allows to recognize pooling problem structures in general mixed integer nonlinear programming problems.

Although the pooling problem has been studied for decades, it was only proved to be strongly NP-hard in 2013 by Alfaki and Haugland [[3](#)]. Further complexity results on special cases of the pooling problem can be found in [[7](#), [9](#), [20](#)].

Haverly [[21](#)] introduced the pooling problem using what is now known as the  $p$ -formulation. Almost 20 years later, Ben-Tal et al. [[8](#)] proposed an equivalent formulation called  $q$ -formulation. Finally, the  $pq$ -formulation was introduced in [[30](#), [34](#)] and is a strengthening of the  $q$ -formulation. It has been shown to be the strongest known formulation for the pooling problem [[34](#)]; i.e., the “natural relaxation” of this formulation  $pq$ -formulation yields a bound on the optimal value that is at least as good as that of any other known formulation.

Many other approaches for solving the pooling problem have been proposed, including: recursive and successive linear programming [[6](#), [21](#)], decomposition methods [[14](#)], and global optimization [[15](#)]. More recently, Dey and Gupte [[13](#)] used discretization strategies to design an approximation algorithm and an effective heuristic. Several variants of the standard pooling problem have been studied, see, for example, [[4](#), [27](#), [29](#), [32](#)]. Some of the variants introduce binary variables to model design decisions, thus yielding a mixed-integer nonlinear programming problem, see, for example, [[11](#), [26](#), [28](#), [35](#)]. For more comprehensive reviews of the pooling problem the reader is referred to [[17](#), [18](#), [27](#), [34](#)] and to [[19](#)] for an overview on the relaxations and discretizations for the pooling problem.

**Notation.** For a set  $T$ ,  $\text{conv}(T)$  denotes the convex hull of  $T$ , and for a convex set  $R$ ,  $\text{ext}(R)$  denotes the set of extreme points of  $R$ .

**2. Mathematical Formulation and Relaxation.** There are multiple formulations for the pooling problem, primarily differing in the modeling of the concentrations of attributes throughout the network. We base our work on the state-of-the-art  $pq$ -formulation.

We are given a directed graph  $G = (V, A)$  where  $V$  is the set of vertices that is partitioned into inputs  $I$ , pools  $L$ , and outputs  $J$ , i.e.,  $V = I \cup L \cup J$ . For a node  $u \in V$ , the sets  $I_u \subseteq I$ ,  $L_u \subseteq L$ ,  $J_u \subseteq J$  denote the inputs, pools, and outputs, respectively, that are directly connected to  $u$ . Arcs  $(i, j) \in A$  link inputs to pools, pools to outputs, and inputs directly to outputs, i.e.,  $A \subseteq (I \times L) \cup (L \times J) \cup (I \times J)$ . In particular, pool-to-pool connections are not considered.

The  $pq$ -formulation of the pooling problem uses the following decision variables:

- $x_{ij}$  is the flow on  $(i, j) \in A$ ;
- $q_{i\ell}$  is the proportion of flow to pool  $\ell \in L$  that comes from input  $i \in I_\ell$ ;
- $w_{i\ell j}$  is the flow from  $i \in I$  through pool  $\ell \in L_i$  to output  $j \in J_\ell$ .

With these definitions, the  $pq$ -formulation of the pooling problem is:

$$\begin{aligned}
(1a) \quad & \min \sum_{(i,j) \in A} c_{ij} x_{ij} \\
(1b) \quad & \text{s.t.} \quad \sum_{\ell \in L_i} x_{i\ell} + \sum_{j \in J_i} x_{ij} \leq C_i && \text{for all } i \in I \\
(1c) \quad & \sum_{j \in J_\ell} x_{\ell j} \leq C_\ell && \text{for all } \ell \in L \\
(1d) \quad & \sum_{\ell \in L_j} x_{\ell j} + \sum_{i \in I_j} x_{ij} \leq C_j && \text{for all } j \in J \\
(1e) \quad & \sum_{i \in I_\ell} q_{i\ell} = 1 && \text{for all } \ell \in L \\
(1f) \quad & w_{i\ell j} = q_{i\ell} x_{\ell j} && \text{for all } i \in I_\ell, \ell \in L_j, j \in J \\
(1g) \quad & x_{i\ell} = \sum_{j \in J_\ell} w_{i\ell j} && \text{for all } i \in I_\ell, \ell \in L \\
(1h) \quad & \sum_{i \in I_j} \bar{\gamma}_{ijk} x_{ij} + \sum_{\ell \in L_j} \sum_{i \in I_\ell} \bar{\gamma}_{ijk} w_{i\ell j} \leq 0 && \text{for all } j \in J, k \in K \\
(1i) \quad & \sum_{i \in I_\ell} w_{i\ell j} = x_{\ell j} && \text{for all } j \in J_\ell, \ell \in L \\
(1j) \quad & \sum_{j \in J_\ell} w_{i\ell j} \leq C_\ell q_{i\ell} && \text{for all } i \in I_\ell, \ell \in L \\
(1k) \quad & 0 \leq x_{ij} \leq C_{ij} && \text{for all } (i, j) \in A \\
(1l) \quad & 0 \leq q_{i\ell} \leq 1 && \text{for all } i \in I_\ell, \ell \in L.
\end{aligned}$$

The objective (1a) is to minimize the production cost, where  $c_{ij}$  is the cost per unit flow on arc  $(i, j)$ . Inequalities (1b)–(1d) represent capacity constraints on inputs, pools, and outputs, respectively, where here  $C_i, i \in I$ ,  $C_\ell, \ell \in L$ , and  $C_j, j \in J$  are given capacity limits. Equations (1e) enforce that the proportions at each pool sum up to one. Equations (1f) and (1g) define the auxiliary variables  $w_{i\ell j}$  and link them to the flow variables. (1h) formulates the quality constraints for each attribute  $k$  in the set of attributes  $K$ . The coefficients  $\bar{\gamma}_{ijk}$  represent the excess of attribute quality  $k$  of the material from input  $i$  with respect to the upper quality bound at output  $j$ . The upper quality bound is met when there is no excess, i.e., the total excess is not positive. For brevity, we do not include lower bounds on attribute quality at the final products, but these can be easily added. Inequalities (1i) and (1j) are redundant in the formulation but are not when the nonconvex constraints (1f) are not enforced as is done in a relaxation-based solution algorithm. These two constraints constitute the difference between the  $q$ - and the  $pq$ -formulation and are responsible for the strong linear relaxation of the latter. Finally, (1k) limits the flow on each arc  $(i, j)$  to a given capacity  $C_{ij}$ .

A linear programming relaxation of the  $pq$ -formulation is obtained by replacing the constraints (1f) with the McCormick inequalities derived using the bounds (1k) and (1l):

$$\begin{aligned}
(2a) \quad & w_{i\ell j} \leq x_{\ell j}, \quad w_{i\ell j} \leq C_\ell q_{i\ell}, && \text{for all } i \in I_\ell, \ell \in L_j, j \in J \\
(2b) \quad & w_{i\ell j} \geq 0, \quad w_{i\ell j} \geq C_\ell q_{i\ell} + x_{\ell j} - C_\ell, && \text{for all } i \in I_\ell, \ell \in L_j, j \in J.
\end{aligned}$$

We refer to the relaxation obtained by replacing (1f) with (2) as the *McCormick relaxation*. Our goal is to derive tighter relaxations of the pooling problem by considering more of the problem structure.

**3. Strong Convex Nonlinear Relaxations.** To derive a stronger relaxation of the pooling problem, we seek to identify a relaxed set that contains the feasible region of the pooling problem, but includes some of the key nonconvex structure. First, we consider only one single attribute  $k \in K$  and relax all constraints (1h) concerning the other attributes. Next, we consider only one output  $j \in J$ , and remove all nodes and arcs which are not in a path to output  $j$ . In particular, this involves all other outputs. Then, we focus on pool  $\ell \in L$  with the intention to split flows into two categories: the flow through pool  $\ell$  and aggregated flow on all paths not passing through pool  $\ell$ , also called “by-pass” flow. Finally, we aggregate all the flow from the inputs to pool  $\ell$ .

As a result, we are left with five decision variables:

1. the total flow through the pool, i.e., the flow  $x_{\ell j}$  from pool  $\ell$  to output  $j$
2. the total flow  $z_{\ell j}$  over the by-pass, i.e., the flow to output  $j$  that does not pass through pool  $\ell$

$$z_{\ell j} := \sum_{i \in I_j} x_{ij} + \sum_{\ell' \in L_j | \ell' \neq \ell} x_{\ell' j}$$

3. the contribution  $u_{k\ell j}$  of the flow through pool  $\ell$  to the excess of attribute  $k$  at output  $j$ , i.e.,

$$u_{k\ell j} := \sum_{i \in I_\ell} \gamma_{kij} w_{ilj}$$

4. the contribution  $y_{k\ell j}$  of by-pass flow to the excess of attribute  $k$  at output  $j$ , i.e.,

$$y_{k\ell j} := \sum_{i \in I_j} \gamma_{kij} x_{ij} + \sum_{\ell' \in L_j | \ell' \neq \ell} \sum_{i \in I_{\ell'}} \gamma_{kij} w_{i\ell' j}$$

5. the attribute quality  $t_{k\ell j}$  of the flow through pool  $\ell$ , i.e.,

$$t_{k\ell} := \sum_{i \in I_\ell} \gamma_{kij} q_{il}$$

With these decision variables, the quality constraint associated with attribute  $k$  of output  $j$  and the capacity constraint associated with output  $j$  from (1) can be written as:

$$(3a) \quad y_{k\ell j} + u_{k\ell j} \leq 0, \quad \text{for all } k \in K, j \in J$$

$$(3b) \quad z_{\ell j} + x_{\ell j} \leq C_j, \quad \text{for all } j \in J.$$

A key property of these new decision variables is the relationship between the flow and quality in the pool with the excess of the attribute contributed by the flow through the pool

$$(4) \quad u_{k\ell j} = x_{\ell j} t_{k\ell} \quad \text{for all } \ell \in L, j \in J,$$

which is valid because using (1f) and (1i)

$$u_{k\ell j} = \sum_{i \in I_\ell} \gamma_{kij} w_{ilj} = \sum_{i \in I_\ell} \gamma_{kij} q_{il} x_{\ell j} = \sum_{i \in I_\ell} \gamma_{kij} q_{il} \sum_{i' \in I_\ell} w_{i'\ell j} = t_{k\ell} x_{\ell j}.$$

In order to derive bounds on the new decision variables we define the parameters  $\underline{\gamma}_{k\ell}$  and  $\bar{\gamma}_{k\ell}$  representing bounds on the excess of attribute  $k$  over inputs that are connected to pool  $\ell$ , and  $\underline{\beta}_{k\ell j}$  and  $\bar{\beta}_{k\ell j}$  representing bounds on the excess of attribute  $k$  over inputs that are connected to output  $j$  via a by-pass flow :

$$\begin{aligned}\underline{\gamma}_{k\ell} &= \min_{i \in I_\ell} \gamma_{ki} & \underline{\beta}_{k\ell j} &= \min\{\gamma_{ki} : i \in I_j \cup \bigcup_{\ell' \in L \setminus \{\ell\}} I_{\ell'}\} \\ \bar{\gamma}_{k\ell} &= \max_{i \in I_\ell} \gamma_{ki} & \bar{\beta}_{k\ell j} &= \max\{\gamma_{ki} : i \in I_j \cup \bigcup_{\ell' \in L \setminus \{\ell\}} I_{\ell'}\}.\end{aligned}$$

We thus have,

$$\begin{aligned}(5a) \quad & t_{k\ell} \in [\underline{\gamma}_{k\ell}, \bar{\gamma}_{k\ell}] && \text{for all } k \in K, \ell \in L \\ (5b) \quad & \underline{\beta}_{k\ell j} z_{\ell j} \leq y_{k\ell j} \leq \bar{\beta}_{k\ell j} z_{\ell j}, && \text{for all } k \in K, \ell \in L, j \in J.\end{aligned}$$

Despite the many relaxations performed in deriving this set, the nonconvex relation (4), which relates the contribution of the excess from the pool to the attribute quality of the pool and the quantity passing through the pool, still preserves a key nonconvex structure of the problem.

With these variables and constraints we now formulate the relaxation of the pooling problem that we study. To simplify notation, we drop the fixed indices  $\ell, j$ , and  $k$ . Gathering the constraints (3), (4), and (5), together with nonnegativity on the  $z$  and  $x$  variable, we define the set  $T$  as those  $(x, u, y, z, t) \in \mathbb{R}^5$  that satisfy:

$$\begin{aligned}(6) \quad & u = xt \\ (7) \quad & y + u \leq 0 \\ (8) \quad & z + x \leq C \\ (9) \quad & y \leq \bar{\beta}z \\ (10) \quad & y \geq \underline{\beta}z \\ & z \geq 0, x \in [0, C], t \in [\underline{\gamma}, \bar{\gamma}].\end{aligned}$$

We can assume, without loss of generality, that  $C = 1$  by scaling the variables  $x, u, y$ , and  $z$  by  $C^{-1}$ .

Due to the nonlinear equation  $u = xt$ ,  $T$  is a nonconvex set unless  $x$  or  $t$  is fixed. Using the bounds  $0 \leq x \leq 1$  and  $\underline{\gamma} \leq t \leq \bar{\gamma}$ , the constraint  $u = xt$  can be relaxed by the McCormick inequalities [25]:

$$\begin{aligned}(11) \quad & u - \underline{\gamma}x \geq 0 \\ (12) \quad & \bar{\gamma}x - u \geq 0 \\ (13) \quad & u - \underline{\gamma}x \leq t - \underline{\gamma} \\ (14) \quad & \bar{\gamma}x - u \leq \bar{\gamma} - t.\end{aligned}$$

Equations (11)–(14) provide the best possible convex relaxation of the feasible points of  $u = xt$  given that  $x$  and  $t$  are in the bounds mentioned above. However, replacing the nonconvex constraint  $u = xt$  with these inequalities is not sufficient to define  $\text{conv}(T)$ .

Note that (11)–(14) imply the bounds  $0 \leq x \leq 1$  and  $\underline{\gamma} \leq t \leq \bar{\gamma}$ . Also the bound constraint  $z \geq 0$  is implied by (9) and (10). Thus, we define the standard relaxation of the set  $T$  by

$$R^0 := \{(x, u, y, z, t) : (7)\text{--}(14)\}.$$

Every convex set is described completely by its extreme points and rays. The set  $T$  is bounded and so has no extreme rays. In [24], we have characterized the extreme points of  $T$ , showing they are not finite. Thus, the convex hull of  $T$  is not a polyhedron.

**3.1. Valid Inequalities.** We now present the new valid inequalities for  $\text{conv}(T)$ , two of them linear, and two of them convex nonlinear. Depending on the signs of  $\underline{\gamma}$  and  $\overline{\gamma}$ , some of these inequalities are redundant. In the following, an inequality is said to be *valid* for a set if every point in the set satisfies the inequality.

**THEOREM 1.** *If  $\underline{\beta} < 0$ , then the following inequality is valid for  $T$ :*

$$(15) \quad (u - \underline{\beta}x)(u - \underline{\gamma}x) \leq -\underline{\beta}x(t - \underline{\gamma})$$

*Proof.* Aggregating the inequalities (7) (with weight 1), (8) (with weight  $-\underline{\beta}$ ), and (10) (with weight 1) yields the inequality  $u - \underline{\beta}x \leq -\underline{\beta}$ , which is valid for  $R^0$ . Multiplying this inequality by  $x(t - \underline{\gamma}) \geq 0$  on both sides yields the nonlinear inequality

$$(u - \underline{\beta}x)x(t - \underline{\gamma}) \leq (-\underline{\beta})x(t - \underline{\gamma})$$

which is also valid for  $R^0$ . Substituting  $u = xt$  into the left-hand-side of this yields (15).  $\square$

We observe that if  $\overline{\gamma} < 0$ , then (15) is redundant. Indeed,  $\overline{\gamma} < 0$  implies  $t < 0$  and therefore  $u < 0$ , which in turn implies  $u - \underline{\beta}x < -\underline{\beta}x$ . On the other hand,  $x \leq 1$  and  $t - \underline{\gamma} > 0$  imply that  $t - \underline{\gamma} \geq xt - \underline{\gamma}x = u - \underline{\gamma}x$ . Furthermore,  $0 = u - xt \leq u - \underline{\gamma}x$  and  $-\underline{\beta}x \geq 0$ . Thus, we conclude that (15) is always strict if  $\overline{\gamma} < 0$ :

$$(u - \underline{\beta}x)(u - \underline{\gamma}x) < -\underline{\beta}x(u - \underline{\gamma}x) \leq -\underline{\beta}x(t - \underline{\gamma}).$$

We next show that (15) is second-order cone representable and thus convex. We can rewrite (15) as:

$$\begin{aligned} (u - \underline{\beta}x)(u - \underline{\gamma}x) \leq -\underline{\beta}x(t - \underline{\gamma}) &\Leftrightarrow (u - \underline{\gamma}x)^2 + (\underline{\gamma} - \underline{\beta})x(u - \underline{\gamma}x) \leq -\underline{\beta}x(t - \underline{\gamma}) \\ &\Leftrightarrow (u - \underline{\gamma}x)^2 \leq x \left[ (-\underline{\beta})(t - \underline{\gamma}) + (\underline{\beta} - \underline{\gamma})(u - \underline{\gamma}x) \right]. \end{aligned}$$

This inequality has the form of a rotated second-order cone,  $2x_1x_2 \geq x_3^2$ , where  $x_1 = x/2$ ,  $x_2 = (-\underline{\beta})(t - \underline{\gamma}) + (\underline{\beta} - \underline{\gamma})(u - \underline{\gamma}x)$ , and  $x_3 = u - \underline{\gamma}x$ . Clearly,  $x_1 \geq 0$ . The following lemma shows the nonnegativity of  $x_2$  and therefore establishes the second-order cone representability of (15).

**LEMMA 2.** *If  $\underline{\beta} < 0$ , the following inequality is valid for  $T$ :*

$$(16) \quad (-\underline{\beta})(t - \underline{\gamma}) + (\underline{\beta} - \underline{\gamma})(u - \underline{\gamma}x) \geq 0$$

*Proof.* First, as  $\underline{\beta} < 0$  then by  $y + u \leq 0$ ,  $-\underline{\beta}(x + z) \leq -\underline{\beta}$ ,  $\underline{\beta}z - y \leq 0$ , and  $\underline{\gamma}x - u \leq 0$ , we have  $(\underline{\gamma} - \underline{\beta})x \leq -\underline{\beta}$ , and therefore, using  $t - \underline{\gamma} \geq 0$ ,

$$(17) \quad (\underline{\gamma} - \underline{\beta})(t - \underline{\gamma})x \leq (-\underline{\beta})(t - \underline{\gamma}).$$

But then, using  $u = tx$ , yields

$$(\underline{\gamma} - \underline{\beta})(t - \underline{\gamma})x = (\underline{\gamma} - \underline{\beta})(tx - \underline{\gamma}x) = (\underline{\gamma} - \underline{\beta})(u - \underline{\gamma}x).$$

Substituting into (17) and rearranging yields the result.  $\square$

The second inequality we derive is valid for points in  $T$  with  $y > 0$ .

**THEOREM 3.** *If  $\bar{\beta} > 0$  and  $\underline{\gamma} < 0$ , then the following inequality is valid for  $T$  when  $y > 0$ :*

$$(18) \quad (\bar{\gamma} - \underline{\gamma})y + \bar{\beta}(\bar{\gamma}x - u) + \frac{\underline{\gamma}y(u - \underline{\gamma}x)}{y + u - \underline{\gamma}x} \leq \bar{\beta}(\bar{\gamma} - t)$$

*Proof.* First, adding (8) scaled by weight  $\bar{\beta} > 0$  to (9) yields the inequality

$$(19) \quad y + \bar{\beta}x \leq \bar{\beta}$$

which is valid for  $R^0$ .

Next, using the substitution  $u = xt$  the left-hand-side of (18) becomes:

$$\begin{aligned} & (\bar{\gamma} - \underline{\gamma})y + \bar{\beta}(\bar{\gamma}x - u) + \frac{\underline{\gamma}y(u - \underline{\gamma}x)}{y + u - \underline{\gamma}x} \\ &= (\bar{\gamma} - \underline{\gamma})y + \bar{\beta}x(\bar{\gamma} - t) + \frac{\underline{\gamma}yx(t - \underline{\gamma})}{y + x(t - \underline{\gamma})} \\ &\leq (\bar{\gamma} - \underline{\gamma})y + \bar{\beta}x(\bar{\gamma} - t) + \frac{\underline{\gamma}yx(t - \underline{\gamma})}{-xt + x(t - \underline{\gamma})} \quad (y \leq -xt \text{ and } \underline{\gamma}yx(t - \underline{\gamma}) \leq 0) \\ &= (\bar{\gamma} - \underline{\gamma})y + \bar{\beta}x(\bar{\gamma} - t) - y(t - \underline{\gamma}) \\ &= \bar{\beta}x(\bar{\gamma} - t) + y(\bar{\gamma} - t) \\ &= (\bar{\beta}x + y)(\bar{\gamma} - t) \leq \bar{\beta}(\bar{\gamma} - t) \quad \text{because } \bar{\gamma} \geq t \text{ and by (19). } \quad \square \end{aligned}$$

The conditional constraint (18) cannot be directly used in an algebraic formulation. We thus derive a convex reformulation for (18) that is valid also for  $y \leq 0$ . To this end define the function  $h : \mathbb{R} \times \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}$  as

$$h(y, v) := \begin{cases} 0 & \text{if } y \leq 0 \\ (\bar{\gamma} - \underline{\gamma})y + \underline{\gamma}g(y, v) & \text{if } y > 0. \end{cases}$$

where

$$g(y, v) := \frac{yv}{y + v}.$$

We next show that  $h$  is convex, and with  $v = u - \underline{\gamma}x$ , can be used to define a constraint equivalent to (18).

**LEMMA 4.** *If  $\bar{\beta} > 0$  and  $\underline{\gamma} < 0$ , then the inequality*

$$(20) \quad \bar{\beta}(\bar{\gamma}x - u) + h(y, u - \underline{\gamma}x) \leq \bar{\beta}(\bar{\gamma} - t)$$

*is valid for  $T$ ,  $h$  is convex over  $\mathbb{R} \times \mathbb{R}_{\geq 0}$ , and any point  $(x, u, y, t)$  with  $y > 0$  satisfies (20) if and only if it satisfies (18).*

*Proof.* The statement that any point with  $y > 0$  satisfies (20) if and only if it satisfies (18) is immediate from the definition of  $h$ .

By **Theorem 3**, inequality (20) is satisfied by all points in  $T$  with  $y > 0$ . If  $y \leq 0$  the inequality is also valid since

$$\bar{\beta}(\bar{\gamma}x - u) + h(y, u, x) = \bar{\beta}(\bar{\gamma}x - u) = x\bar{\beta}(\bar{\gamma} - t) \leq \bar{\beta}(\bar{\gamma} - t).$$

We next show that  $g$  is concave over  $\mathbb{R}_{>0} \times \mathbb{R}_{\geq 0}$ . We use the python library Sympy [33] to compute the Hessian of  $g$ , and obtain

$$\begin{pmatrix} \frac{2vy}{(v+y)^3} - \frac{2y}{(v+y)^2} & \frac{2vy}{(v+y)^3} - \frac{v}{(v+y)^2} - \frac{y}{(v+y)^2} + \frac{1}{v+y} \\ \frac{2vy}{(v+y)^3} - \frac{v}{(v+y)^2} - \frac{y}{(v+y)^2} + \frac{1}{v+y} & \frac{2vy}{(v+y)^3} - \frac{2v}{(v+y)^2} \end{pmatrix}$$

and its Eigenvalues as  $\lambda_1 = 0$  and  $\lambda_2 = -(2v^2 + 2y^2)/(v+y)^3$ . The second Eigenvalue  $\lambda_2$  is negative because  $v \geq 0$ ,  $y > 0$ . The Hessian is therefore negative semidefinite and  $g$  is concave.

Finally, we show that  $h$  is convex. Let  $p_i = (y_i, v_i) \in \mathbb{R} \times \mathbb{R}_{\geq 0}$  for  $i = 1, 2$  and  $\lambda \in (0, 1)$ . We need to show that

$$(21) \quad h(\lambda p_1 + (1 - \lambda)p_2) \leq \lambda h(p_1) + (1 - \lambda)h(p_2).$$

If  $y_i > 0$ ,  $i = 1, 2$ , then (21) holds because  $g$  is concave over  $\mathbb{R}_{>0} \times \mathbb{R}_{\geq 0}$ , and hence because  $\underline{\gamma} < 0$ ,  $h$  is convex over this region. If  $y_i \leq 0$ ,  $i = 1, 2$ , then (21) holds because  $\bar{h}$  is linear over the points with  $y \leq 0$ . Therefore, assume without loss of generality  $y_1 \leq 0$  and  $y_2 > 0$ . First we show that  $h$  is nonnegative. For  $y \leq 0$  this is clear and for  $y > 0$  we have

$$h(u, v) = (\bar{\gamma} - \underline{\gamma})y + \frac{\underline{\gamma}yv}{y+v} = \frac{(\bar{\gamma} - \underline{\gamma})y(y+v) + \underline{\gamma}yv}{y+v} = \frac{(\bar{\gamma} - \underline{\gamma})y^2 + \bar{\gamma}yv}{y+v} \geq 0.$$

Furthermore we know  $h(p_1) = 0$  since  $y_1 \leq 0$ . If  $h(\lambda p_1 + (1 - \lambda)p_2) = 0$ , then (21) is always fulfilled. If  $h(\lambda p_1 + (1 - \lambda)p_2)$  does not vanish, then denote by  $p_3 = (y_3, v_3)$  the point on the line between  $p_1$  and  $p_2$  with  $y_3 = 0$ . If  $v_3 = 0$ , then  $v_2 = 0$  since  $v_1 \geq 0$ . In this case  $g$  vanishes such that  $h$  is linear between  $p_3$  and  $p_2$  and (21) is fulfilled. If  $v_3 > 0$ , then  $g$  is also well-defined at  $p_3$  with  $g(p_3) = 0$  so that  $h(p_3) = (\bar{\gamma} - \underline{\gamma})y_3 + \underline{\gamma}g(p_3) = 0$  and  $h$  is convex on the line between  $p_3$  and  $p_2$ . Furthermore, there exists a  $\hat{\lambda}$  such that

$$\lambda p_1 + (1 - \lambda)p_2 = \hat{\lambda} p_3 + (1 - \hat{\lambda})p_2$$

and since  $p_3$  is closer to  $p_2$  than  $p_1$ , it holds that  $\lambda \leq \hat{\lambda}$ . Finally, we can show that (21) also holds in this case:

$$\begin{aligned} h(\lambda p_1 + (1 - \lambda)p_2) &= h(\hat{\lambda} p_3 + (1 - \hat{\lambda})p_2) \\ &\leq \hat{\lambda} h(p_3) + (1 - \hat{\lambda})h(p_2) \\ &= \lambda h(p_1) + (1 - \hat{\lambda})h(p_2) \leq \lambda h(p_1) + (1 - \lambda)h(p_2). \quad \square \end{aligned}$$

The remaining two new valid inequalities we present are linear.

**THEOREM 5.** *If  $\bar{\beta} > 0$ , then the following inequality is valid for  $T$ :*

$$(22) \quad (\bar{\gamma} - \underline{\gamma})y + \underline{\gamma}(\bar{\gamma}x - u) + \bar{\beta}(u - \underline{\gamma}x) \leq \bar{\beta}(t - \underline{\gamma}).$$

*Proof.* First observe that  $y + u \leq 0$  and  $-u \leq -\underline{\gamma}x$  together imply

$$(23) \quad y \leq -x\underline{\gamma}.$$

Next,

$$(\bar{\gamma} - \underline{\gamma})y = (t - \underline{\gamma})y + (\bar{\gamma} - t)y$$



$$\begin{aligned}
&\leq (t - \underline{\gamma})\bar{\beta}z + (\bar{\gamma} - t)y && \text{because } y \leq \bar{\beta}z \text{ and } t - \underline{\gamma} \geq 0 \\
&\leq (t - \underline{\gamma})\bar{\beta}z + (\bar{\gamma} - t)(-x\underline{\gamma}) && \text{by (23) and } \bar{\gamma} - t \geq 0
\end{aligned}$$

and thus

$$(24) \quad (\bar{\gamma} - \underline{\gamma})y - (t - \underline{\gamma})\bar{\beta}z + (\bar{\gamma} - t)(x\underline{\gamma}) \leq 0.$$

Then, multiply the inequality  $z + x \leq 1$  on both sides by  $\bar{\beta}(t - \underline{\gamma}) \geq 0$  to yield:

$$(25) \quad (t - \underline{\gamma})\bar{\beta}z + (t - \underline{\gamma})\bar{\beta}x \leq (t - \underline{\gamma})\bar{\beta}$$

Adding (24) and (25) yields:

$$(26) \quad (\bar{\gamma} - \underline{\gamma})y + (\bar{\gamma} - t)x\underline{\gamma} + (t - \underline{\gamma})\bar{\beta}x \leq (t - \underline{\gamma})\bar{\beta}$$

Finally, substituting  $u = xt$  from (6) yields (22).  $\square$

We next show that if  $\bar{\gamma} > 0$ , then (22) is redundant. Assuming  $\bar{\gamma} > 0$ , then scaling the inequality  $-u + \underline{\gamma}x \leq 0$  by  $\bar{\gamma} > 0$  and combining that with the valid inequality  $(\bar{\gamma} - \underline{\gamma})y + (\bar{\gamma} - \underline{\gamma})u \leq 0$  and yields

$$(27) \quad (\bar{\gamma} - \underline{\gamma})y - \underline{\gamma}u + \underline{\gamma}\bar{\gamma}x \leq 0.$$

But, also since  $u - \underline{\gamma}x \leq t - \underline{\gamma}$ , it follows that  $\bar{\beta}(u - \underline{\gamma}x) \leq \bar{\beta}(t - \underline{\gamma})$ . Combining this with (27) implies (22).

The next theorem presents the last valid inequality for  $T$  in this section.

**THEOREM 6.** *If  $\underline{\beta} < 0$ , then the following inequality is valid for  $T$ :*

$$(28) \quad (\underline{\gamma} - \underline{\beta})(\bar{\gamma}x - u) \leq -\underline{\beta}(\bar{\gamma} - t).$$

*Proof.* Aggregate inequality (8) with weight  $-\underline{\beta} > 0$  yields

$$(29) \quad -\underline{\beta}(z + x) \leq -\underline{\beta}.$$

Furthermore, using  $y \geq \underline{\beta}z$ ,  $\underline{\beta} < 0$ , and (23), yields  $-\underline{\beta}z + x\underline{\gamma} \leq 0$ , which combined with (29) yields

$$(\underline{\gamma} - \underline{\beta})x \leq -\underline{\beta}.$$

Multiplying both sides of this inequality by  $\bar{\gamma} - t \geq 0$  yields

$$(\underline{\gamma} - \underline{\beta})x(\bar{\gamma} - t) \leq -\underline{\beta}(\bar{\gamma} - t).$$

Substituting  $xt = u$  yields (28).  $\square$

If  $\underline{\gamma} < 0$ , then  $(\underline{\gamma} - \underline{\beta})(\bar{\gamma}x - u) \leq -\underline{\beta}(\bar{\gamma}x - 0) \leq -\underline{\beta}(\bar{\gamma} - t)$  and so (28) is redundant.

**4. Convex hull analysis.** We next demonstrate that the set  $R^0$  combined with certain subsets of the new valid inequalities, depending on the sign of  $\underline{\gamma}$  and  $\bar{\gamma}$ , are sufficient to define the convex hull of  $T$ . Let us first restate the relevant inequalities for convenience:

$$(15) \quad (u - \underline{\beta}x)(u - \underline{\gamma}x) \leq -\underline{\beta}x(t - \underline{\gamma})$$

Result	Used in proof of	Stated on
Lemma 11	Theorems 7 to 9	Page 11
Lemma 14	Theorem 7	Page 12
Lemma 15	Theorem 7	Page 15
Lemma 16	Theorem 8	Page 16
Lemma 17	Theorem 8	Page 17
Lemma 19	Theorem 9	Page 19
Lemma 20	Theorem 9	Page 20

TABLE 1  
Overview over lemmas used in the proofs of Theorems 7 to 9

$$(18) \quad (\bar{\gamma} - \underline{\gamma})y + \bar{\beta}(\bar{\gamma}x - u) + \frac{\gamma y(u - \underline{\gamma}x)}{y + u - \underline{\gamma}x} \leq \bar{\beta}(\bar{\gamma} - t) \quad \text{if } y > 0.$$

$$(22) \quad (\bar{\gamma} - \underline{\gamma})y + \underline{\gamma}(\bar{\gamma}x - u) + \bar{\beta}(u - \underline{\gamma}x) \leq \bar{\beta}(t - \underline{\gamma})$$

$$(28) \quad (\underline{\gamma} - \underline{\beta})(\bar{\gamma}x - u) \leq -\underline{\beta}(\bar{\gamma} - t).$$

Next, we define the sets which include the nonredundant valid inequalities for different signs of  $\underline{\gamma}$  and  $\bar{\gamma}$ :

$$R^1 = \{(x, u, y, z, t) \in R^0 : (15) \text{ and } (18)\},$$

$$R^2 = \{(x, u, y, z, t) \in R^0 : (18) \text{ and } (22)\},$$

$$R^3 = \{(x, u, y, z, t) \in R^0 : (15) \text{ and } (28)\}.$$

The following theorems show that  $R^1, R^2$ , and  $R^3$  describe the convex hull of  $T$  in different cases. Since all inequalities that define the sets are valid for  $T$  and convex,  $R^i$  are convex relaxations for  $T$  and we know  $\text{conv}(T) \subseteq R^i$  for  $i = 1, 2, 3$ . To show that a relaxation defines  $\text{conv}(T)$  in a particular case, we show that every extreme point of the relaxation satisfies the nonconvex constraint  $u = xt$  even though this equation is not enforced in the relaxation. The three main theorems are stated next, and are proved using lemmas that are stated and proved thereafter. Table 1 gives an overview of which of the lemmas is used in the proof of each theorem and on which page the lemmas are found.

**THEOREM 7.** Assume  $\underline{\gamma} < 0 < \bar{\gamma}$  and  $\underline{\beta} < 0 < \bar{\beta}$ . Then  $\text{conv}(T) = R^1$ .

*Proof.* Being a bounded convex set,  $R^1$  is completely characterized by its extreme points. We prove that every extreme point of  $R^1$  is in  $T$ , i.e., fulfills the equation  $u = xt$ . Every point in  $R^1$  can thus be represented as a convex combination of points in  $T$  and  $R^1 = \text{conv}(T)$  is proved.

It remains to show that  $u = xt$  for all  $p = (x, u, y, z, t) \in \text{ext}(R^1)$ . Lemma 11 shows that this is the case for  $x$  or  $t$  are at its bounds, i.e., if  $x \in \{0, 1\}$  or  $t \in \{\underline{\gamma}, \bar{\gamma}\}$ . Under the condition  $0 < x < 1$  and  $\underline{\gamma} < t < \bar{\gamma}$ , Lemmas 14 and 15 show that points with  $u < xt$  and  $u > xt$ , respectively, cannot be extreme.  $\square$

**THEOREM 8.** Assume  $\underline{\gamma} < \bar{\gamma} < 0$  and  $\underline{\beta} < 0 < \bar{\beta}$ . Then  $\text{conv}(T) = R^2$ .

*Proof.* Based on the same argument as in the proof of Theorem 7, we show that that  $u = xt$  for all  $p = (x, u, y, z, t) \in \text{ext}(R^2)$ . Lemma 11 shows that for  $x \in \{0, 1\}$  or  $t \in \{\underline{\gamma}, \bar{\gamma}\}$ . For  $0 < x < 1$  and  $\underline{\gamma} < t < \bar{\gamma}$  and under the assumptions of this theorem

Lemmas 16 and 17 show that points with  $u < xt$  and  $u > xt$ , respectively, cannot be extreme.  $\square$

THEOREM 9. Assume  $0 < \underline{\gamma} < \bar{\gamma}$  and  $\underline{\beta} < 0 < \bar{\beta}$ . Then  $\text{conv}(T) = R^3$ .

*Proof.* The proof is analogous to the proofs of Theorems 7 and 8, but in this case Lemmas 19 and 20 show that points with  $u < xt$  and  $u > xt$ , respectively, cannot be extreme.  $\square$

**4.1. Preliminary Results.** In the following, for different assumptions on the sign of  $\underline{\gamma}$  and  $\bar{\gamma}$ , we demonstrate that if  $p = (x, u, y, z, t)$  has either  $u > xt$  or  $u < xt$ , then  $p$  is not an extreme point of  $\text{conv}(T)$ . This is accomplished by considering different cases and in each case, we provide two distinct points which depend on a parameter  $\epsilon > 0$ , denoted  $p_i^\epsilon$ ,  $i = 1, 2$ , which satisfy  $p = (1/2)p_1^\epsilon + (1/2)p_2^\epsilon$ . Furthermore, the points  $p_i^\epsilon$  are defined such that  $p_i^\epsilon \rightarrow p$  as  $\epsilon \rightarrow 0$ . The points are then shown to be in the given relaxation for  $\epsilon > 0$  small enough, providing a proof that  $p$  is not an extreme point of the relaxation. To show the points are in a given relaxation for  $\epsilon > 0$  small enough, for each inequality defining the relaxation we either directly show the points satisfy the inequality, or else we show that the point  $p$  satisfies the inequality with strict inequality. In the latter case, the following lemma ensures that both points  $p_1^\epsilon$  and  $p_2^\epsilon$  satisfy the constraint if  $\epsilon$  is small enough.

LEMMA 10. Let  $p^\epsilon : \mathbb{R}_+ \rightarrow \mathbb{R}^n$  with  $\lim_{\epsilon \rightarrow 0} p^\epsilon = p$  for some  $p \in \mathbb{R}^n$ . Suppose  $ap < b$  for  $a \in \mathbb{R}^n$ ,  $b \in \mathbb{R}$ . Then there exists an  $\hat{\epsilon} > 0$  such that

$$ap^\epsilon < b \quad \text{for all } \epsilon < \hat{\epsilon}.$$

*Proof.* Follows directly from continuity of the function  $f(x) = ax - b$ .  $\square$

Throughout this section, for  $\epsilon > 0$ , we use the notation:

$$\alpha_1^\epsilon = 1 - \epsilon, \quad \alpha_2^\epsilon = 1 + \epsilon \quad \text{and} \quad \delta_1^\epsilon = \epsilon, \quad \delta_2^\epsilon = -\epsilon.$$

Obviously,  $\lim_{\epsilon \rightarrow 0} \alpha_i^\epsilon = 1$  and  $\lim_{\epsilon \rightarrow 0} \delta_i^\epsilon = 0$  for  $i \in \{1, 2\}$ .

The series of Lemmas that prove Theorems 7 to 9 is started by Lemma 11 which applies to all cases and tells us that points on the boundaries of the domains of  $x$  and  $t$  fulfill  $u = xt$ .

LEMMA 11. Let  $p = (x, u, y, z, t) \in R^0$ . If  $x = 0$ ,  $x = 1$ ,  $t = \underline{\gamma}$ , or  $t = \bar{\gamma}$ , then  $u = xt$ .

*Proof.* This follows since (11)–(14) are the McCormick inequalities for relaxing the constraint  $u = xt$  over  $x \in [0, 1]$  and  $t \in [\underline{\gamma}, \bar{\gamma}]$ , and it is known (e.g., [2]) that if either of the variables are at its bound, then the McCormick inequalities ensure that  $u = xt$ .  $\square$

As Lemma 11 applies to all the cases we assume from now on that  $0 < x < 1$  and  $\underline{\gamma} < t < \bar{\gamma}$ . We use the following two propositions in several places in this section.

PROPOSITION 12. Suppose  $\underline{\beta} < 0$ . Let  $p = (x, u, y, z, t) \in R^0$  with  $0 < x < 1$  and  $\underline{\gamma} < t < \bar{\gamma}$ .

1. If  $u < xt$ , then  $p$  satisfies (12), (13), and (15) with strict inequality.
2. If  $u > xt$ , then  $p$  satisfies (11) and (14) with strict inequality.

*Proof.* 1. Suppose  $u < xt$ . Then,  $\bar{\gamma}x - u > \bar{\gamma}x - xt = x(\bar{\gamma} - t) > 0$ , and so  $p$  satisfies (12) with strict inequality. Next,

$$(30) \quad u - \underline{\gamma}x < xt - \underline{\gamma}x = x(t - \underline{\gamma}) < t - \underline{\gamma}$$

as  $x < 1$  and  $t > \underline{\gamma}$ , and so (13) is satisfied by  $p$  with strict inequality. To show that (15) is satisfied strictly, we aggregate (7) with weight 1, (8) with weight  $-\underline{\beta}$ , and (10) with weight 1 and get

$$(31) \quad u - \underline{\beta}x \leq -\underline{\beta}.$$

As  $u - \underline{\gamma}x \geq 0$ ,

$$(u - \underline{\beta}x)(u - \underline{\gamma}x) \leq -\underline{\beta}(u - \underline{\gamma}x) < -\underline{\beta}x(t - \underline{\gamma})$$

where the last inequality follows from (30) and  $\underline{\beta} < 0$ , and thus (15) is satisfied by  $p$  with strict inequality.

2. Now suppose  $u > xt$ . Then,  $u - x\underline{\gamma} > xt - x\underline{\gamma} = x(t - \underline{\gamma}) > 0$  and so  $p$  satisfies (11) with strict inequality. Next,

$$(32) \quad \bar{\gamma}x - u < \bar{\gamma}x - xt = x(\bar{\gamma} - t) < \bar{\gamma} - t$$

as  $x < 1$  and  $t < \bar{\gamma}$ , and so (14) is satisfied with strict inequality.  $\square$

**PROPOSITION 13.** *Suppose  $\underline{\beta} < 0$  and  $\underline{\gamma} < 0$ . Let  $p = (x, u, y, z, t) \in R^0$  with  $0 < x < 1$  and  $\underline{\gamma} < t < \bar{\gamma}$ . If  $u > xt$  and  $\underline{y} > 0$ , then  $p$  satisfies (18) with strict inequality.*

*Proof.* Then, as  $\underline{\gamma}y < 0$ , we have

$$\underline{\gamma}y(u - \underline{\gamma}x) < \underline{\gamma}y(xt - \underline{\gamma}x) = \underline{\gamma}yx(t - \underline{\gamma}).$$

Thus, as  $y + u - \underline{\gamma}x > 0$ ,

$$\frac{\underline{\gamma}y(u - \underline{\gamma}x)}{y + u - \underline{\gamma}x} < \frac{\underline{\gamma}yx(t - \underline{\gamma})}{y + u - \underline{\gamma}x} \leq \frac{\underline{\gamma}yx(t - \underline{\gamma})}{-\underline{\gamma}x} = -y(t - \underline{\gamma})$$

where the last inequality follows from  $y + u \leq 0$  and  $\underline{\gamma}yx(t - \underline{\gamma}) < 0$ . Thus,

$$\begin{aligned} (\bar{\gamma} - \underline{\gamma})y + \bar{\beta}(\underline{\gamma}x - u) + \frac{\underline{\gamma}y(u - \underline{\gamma}x)}{y + u - \underline{\gamma}x} &< (\bar{\gamma} - \underline{\gamma})y + \bar{\beta}(\underline{\gamma}x - u) - y(t - \underline{\gamma}) \\ &< y(\bar{\gamma} - t) + \bar{\beta}x(\bar{\gamma} - t) \\ &= (y + \bar{\beta}x)(\bar{\gamma} - t) \leq \bar{\beta}(\bar{\gamma} - t) \end{aligned}$$

where the last inequality follows from  $\bar{\gamma} - t > 0$  and the fact that aggregating (8) with weight  $\bar{\beta}$  and (9) yields  $y + \bar{\beta}x \leq \bar{\beta}$ .  $\square$

**4.2. Proof of Theorem 7.** We now state and prove the two main lemmas that support the proof of Theorem 7.

**LEMMA 14.** *Suppose  $\underline{\beta} < 0 < \bar{\beta}$ . Let  $p = (x, u, y, z, t) \in R^1$  with  $0 < x < 1$  and  $\underline{\gamma} < t < \bar{\gamma}$ . If  $u < xt$ , then  $p$  is not an extreme point of  $R^1$ .*

*Proof.* We consider four cases: (a)  $y + u < 0$ , (b)  $z + x < 1$ , (c)  $\underline{\beta}z - y < 0$  and  $y - \bar{\beta}z < 0$ , and (d)  $z + x = 1$ ,  $y + u = 0$ , and either  $\beta z - y = 0$  or  $y - \bar{\beta}z = 0$ . In each of them we define a series of points  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  for  $i \in \{1, 2\}$  that depends on  $\epsilon > 0$  with  $p = 0.5(p_1^\epsilon + p_2^\epsilon)$  and which satisfy  $\lim_{\epsilon \rightarrow 0} p_i^\epsilon = p$ . We then show that both  $p_i^\epsilon$  are in  $R^1$  and thus  $p$  is not an extreme point of  $R^1$ . To show  $p_i^\epsilon \in R^1$ , we need to ensure that it satisfies all inequalities defining  $R^1$ . For those inequalities that satisfied

strictly at  $p$ , [Lemma 10](#) ensures that this is the case. For the remaining inequalities, we show it directly.

By [Proposition 12](#),  $u < xt$  implies that  $p$  satisfies [\(12\)](#), [\(13\)](#), and [\(15\)](#) with strict inequality. It remains to show that the points  $p_i^\epsilon$  satisfy [\(7\)](#)–[\(11\)](#), [\(14\)](#), and [\(18\)](#) for  $\epsilon > 0$  small enough. Note that  $z \geq 0$  is implied by [\(9\)](#) and [\(10\)](#) and does not have to be proved explicitly.

**Case (a):**  $y + u < 0$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$\begin{aligned} x_i^\epsilon &:= (1 - \alpha_i^\epsilon) + \alpha_i^\epsilon x, & u_i^\epsilon &:= \gamma(1 - \alpha_i^\epsilon) + \alpha_i^\epsilon u, & y_i^\epsilon &:= \alpha_i^\epsilon y, \\ z_i^\epsilon &:= \alpha_i^\epsilon z, & t_i^\epsilon &:= (1 - \alpha_i^\epsilon)\gamma + \alpha_i^\epsilon t. \end{aligned}$$

Since  $\alpha_i^\epsilon$  converge to 1, it is clear that  $p_i^\epsilon$  converges to  $p$  and [Lemma 10](#) can be applied. In the following we check that  $p_i^\epsilon$  satisfies the remaining inequalities.

[\(7\)](#): Satisfied strictly by  $p$  by the assumption of this case.

[\(8\)](#)–[\(10\)](#): Easily checked directly.

[\(11\)](#): Follows from

$$u_i^\epsilon - \gamma x_i^\epsilon = \gamma(1 - \alpha_i^\epsilon) + \alpha_i^\epsilon u - \gamma((1 - \alpha_i^\epsilon) + \alpha_i^\epsilon x) = \alpha_i^\epsilon(u - \gamma x) \geq 0.$$

[\(14\)](#): Follows from

$$\begin{aligned} \bar{\gamma} x_i^\epsilon - u_i^\epsilon &= \bar{\gamma}((1 - \alpha_i^\epsilon) + \alpha_i^\epsilon x) - \gamma(1 - \alpha_i^\epsilon) - \alpha_i^\epsilon u \\ &= (1 - \alpha_i^\epsilon)(\bar{\gamma} - \gamma) + \alpha_i^\epsilon(\bar{\gamma}x - u) \\ &\leq (1 - \alpha_i^\epsilon)(\bar{\gamma} - \gamma) + \alpha_i^\epsilon(\bar{\gamma} - t) = \bar{\gamma} - (1 - \alpha_i^\epsilon)\gamma - \alpha_i^\epsilon t = \bar{\gamma} - t_i^\epsilon. \end{aligned}$$

[\(18\)](#): If  $y > 0$ , then also  $y_i^\epsilon > 0$ , and using  $u_i^\epsilon - \gamma x_i^\epsilon = \alpha_i^\epsilon(u - \gamma x)$  and  $\bar{\gamma} x_i^\epsilon - u_i^\epsilon = (1 - \alpha_i^\epsilon)(\bar{\gamma} - \gamma) + \alpha_i^\epsilon(\bar{\gamma}x - u)$ , the left-hand-side of [\(18\)](#) evaluated at  $p_i^\epsilon$  equals:

$$\begin{aligned} &\alpha_i^\epsilon \left( (\gamma - \bar{\gamma})y + \bar{\beta}(\bar{\gamma}x - u) + \frac{\gamma y(u - \gamma x)}{y + u + \gamma x} \right) + \bar{\beta}(1 - \alpha_i^\epsilon)(\gamma - \bar{\gamma}) \\ &\leq \alpha_i^\epsilon \bar{\beta}(\bar{\gamma} - t) + \bar{\beta}(1 - \alpha_i^\epsilon)(\bar{\gamma} - \gamma) = \bar{\beta}(\bar{\gamma} - \alpha_i^\epsilon t - (1 - \alpha_i^\epsilon)\gamma) = \bar{\beta}(\bar{\gamma} - t_i^\epsilon) \end{aligned}$$

and hence [\(18\)](#) is satisfied by  $p_i^\epsilon$  for  $i = 1, 2$  and any  $\epsilon \in (0, 1)$  when  $y > 0$ . On the other hand, if  $y \leq 0$ , then  $y_i^\epsilon \leq 0$ , and  $p_i^\epsilon$  is not required to satisfy [\(18\)](#) for  $i = 1, 2$ .

**Case (b):**  $z + x < 1$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon := \alpha_i^\epsilon x, \quad u_i^\epsilon := \alpha_i^\epsilon u, \quad y_i^\epsilon := \alpha_i^\epsilon y, \quad z_i^\epsilon := \alpha_i^\epsilon z, \quad t_i^\epsilon := \alpha_i^\epsilon t + (1 - \alpha_i^\epsilon)\bar{\gamma}.$$

[\(7\)](#): Easily checked directly.

[\(8\)](#): Satisfied strictly by  $p$  by the assumption of this case.

[\(9\)](#)–[\(11\)](#): Easily checked directly.

[\(14\)](#): Follows from

$$\bar{\gamma} x_i^\epsilon - u_i^\epsilon = \alpha_i^\epsilon(\bar{\gamma}x - u) \leq \alpha_i^\epsilon(\bar{\gamma} - t) = \alpha_i^\epsilon \bar{\gamma} - \alpha_i^\epsilon t = \alpha_i^\epsilon \bar{\gamma} - (1 - \alpha_i^\epsilon)\bar{\gamma} - t_i^\epsilon = \bar{\gamma} - t_i^\epsilon.$$

[\(18\)](#): If  $y > 0$ , then also  $y_i^\epsilon > 0$ , and the left-hand-side of [\(18\)](#) evaluated at  $p_i^\epsilon$  equals:

$$\alpha_i^\epsilon \left( (\gamma - \bar{\gamma})y + \bar{\beta}(\bar{\gamma}x - u) + \frac{\gamma y(u - \gamma x)}{y + u + \gamma x} \right) \leq \alpha_i^\epsilon \bar{\beta}(\bar{\gamma} - t)$$

$$= \bar{\beta}(\alpha_i^\epsilon \bar{\gamma} - t_i^\epsilon + (1 - \alpha_i^\epsilon) \bar{\gamma}) = \bar{\beta}(\bar{\gamma} - t_i^\epsilon)$$

and hence (18) is satisfied by  $p_i^\epsilon$  for  $i = 1, 2$  and any  $\epsilon \in (0, 1)$  when  $y > 0$ . On the other hand, if  $y \leq 0$ , then  $y_i^\epsilon \leq 0$ , and  $p_i^\epsilon$  is not required to satisfy (18) for  $i = 1, 2$ .

**Case (c):**  $\underline{\beta}z - y < 0$  and  $y - \bar{\beta}z < 0$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where

$$x_i^\epsilon := \alpha_i^\epsilon x, \quad u_i^\epsilon := \alpha_i^\epsilon u, \quad y_i^\epsilon := \alpha_i^\epsilon y, \quad z_i^\epsilon := (1 - \alpha_i^\epsilon) + \alpha_i^\epsilon z, \quad t_i^\epsilon := \alpha_i^\epsilon t + (1 - \alpha_i^\epsilon) \bar{\gamma},$$

for  $i = 1, 2$ .

(7): Easily checked directly.

(8): Follows from

$$z_i^\epsilon + x_i^\epsilon = (1 - \alpha_i^\epsilon) + \alpha_i^\epsilon z + \alpha_i^\epsilon x = (1 - \alpha_i^\epsilon) + \alpha_i^\epsilon (z + x) \leq 1.$$

(9), (10): Satisfied strictly by  $p$  by the assumption of this case.

(11): Easily checked directly.

(14), (18): As the definitions of  $t_i^\epsilon, y_i^\epsilon, x_i^\epsilon$ , and  $u_i^\epsilon$  are the same as in Case (b), it follows from the arguments in that case that  $p_i^\epsilon$  satisfies (14) and (18) for  $i = 1, 2$  and any  $\epsilon \in (0, 1)$ .

**Case (d):**  $z + x = 1, y + u = 0$ , and either  $\underline{\beta}z - y = 0$  or  $y - \bar{\beta}z = 0$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon := x - \delta_i^\epsilon, \quad u_i^\epsilon := u - \underline{\beta} \delta_i^\epsilon, \quad y_i^\epsilon := y + \underline{\beta} \delta_i^\epsilon, \quad z_i^\epsilon := z + \delta_i^\epsilon, \quad t_i^\epsilon := t + \delta_i^\epsilon (\bar{\gamma} - \underline{\beta}).$$

(7), (8): Easily checked directly.

(9): We show that when  $z + x = 1$  and  $y + u = 0$ , then  $y - \bar{\beta}z < 0$ . Indeed, if  $y - \bar{\beta}z = 0$ , then as  $z + x = 1$ , it follows that

$$(33) \quad y + \bar{\beta}x = \bar{\beta}$$

Then, using  $y = \bar{\beta}z > 0$ , and evaluating  $p$  in the left-hand-side of (18) yields

$$\begin{aligned} & (\bar{\gamma} - \underline{\gamma})y + \bar{\beta}(\bar{\gamma}x - u) + \frac{\underline{\gamma}y(u - \underline{\gamma}x)}{y + u - \underline{\gamma}x} \\ &= (\bar{\gamma} - \underline{\gamma})y + \bar{\beta}(\bar{\gamma}x - u) + \frac{\underline{\gamma}y(u - \underline{\gamma}x)}{-\underline{\gamma}x} \quad \text{since } y + u = 0 \\ &= \bar{\gamma}(y + \bar{\beta}x) - u(\bar{\beta} + y/x) \\ &> \bar{\gamma}(y + \bar{\beta}x) - xt(\bar{\beta} + y/x) \quad \text{since } u < xt \text{ and } \bar{\beta} + y/x > 0 \\ &= (\bar{\gamma} - t)(y + \bar{\beta}x) = (\bar{\gamma} - t)\bar{\beta} \quad \text{by (33)}. \end{aligned}$$

Thus,  $p$  violates (18) and hence  $p$  fulfills (9) with strict inequality. Furthermore, due to the assumptions of this case, we can assume  $\underline{\beta}z - y = 0$ .

(10): Easily checked directly.

(11): As  $\underline{\beta}z - y = 0, z > 0$  and  $x > 0$ ,  $p$  satisfies (11) with strict inequality:

$$u - \underline{\gamma}x = -y - \underline{\gamma}x = -\underline{\beta}z - \underline{\gamma}x > 0.$$

(14): Follows from

$$\bar{\gamma}x_i^\epsilon - u_i^\epsilon = \bar{\gamma}x - \bar{\gamma}\delta_i^\epsilon - u + \underline{\beta}\delta_i^\epsilon \leq \bar{\gamma} - t + \delta_i^\epsilon(\underline{\beta} - \bar{\gamma}) = \bar{\gamma} - t_i^\epsilon.$$

(18): Because  $z > 0$  and  $y = \underline{\beta}z < 0$ , it follows that  $y_i^\epsilon < 0$  and  $p_i^\epsilon$  is not subject to (18).  $\square$

LEMMA 15. Suppose  $\bar{\gamma} > 0$  and  $\underline{\beta} < 0 < \bar{\beta}$ . Let  $p = (x, u, y, z, t) \in R^1$  with  $0 < x < 1$  and  $\underline{\gamma} < t < \bar{\gamma}$ . If  $u > xt$  and either  $y \leq 0$  or  $p$  satisfies (18) with strict inequality, then  $p$  is not an extreme point of  $R^1$ .

We first comment that the assumption that either  $y \leq 0$  or  $p$  satisfies (18) with strict inequality follows from the assumption  $u > xt$  and Proposition 13 when  $\gamma < 0$ . However, we state the assumption in this way in order to make the applicability of this proposition clear for a later case when  $\gamma > 0$ .

*Proof.* This proof has the same structure as the proof of Lemma 14. By Proposition 12,  $u > xt$  implies that  $p$  satisfies (11) and (14) with strict inequality. Also, by assumption, if  $y > 0$ , then  $p$  satisfies (18) with strict inequality. It remains to show that the points  $p_i^\epsilon$  satisfy (7)–(10), (12), (13), and (15) for  $\epsilon$  small enough. We consider four cases.

**Case (a):**  $y + u < 0$  and  $z + x = 1$ . Note that  $z + x = 1$  and  $x < 1$  implies that  $z > 0$ . Thus, either (9) or (10) is satisfied strictly by  $p$ . If  $y - \bar{\beta}z < 0$ , define  $y_i^\epsilon := (1 - \alpha_i^\epsilon)\bar{\beta} + \alpha_i^\epsilon y$ , and otherwise, if  $\beta z - y < 0$ , define  $y_i^\epsilon := (1 - \alpha_i^\epsilon)\bar{\beta} + \alpha_i^\epsilon y$  for  $\epsilon > 0$ . Then, for  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon = \alpha_i^\epsilon x, \quad u_i^\epsilon = \alpha_i^\epsilon u, \quad z_i^\epsilon = (1 - \alpha_i^\epsilon) + \alpha_i^\epsilon z, \quad t_i^\epsilon = (1 - \alpha_i^\epsilon)\underline{\gamma} + \alpha_i^\epsilon t.$$

(7): Satisfied strictly by  $p$  by the assumption of this case.

(8): Easily checked directly.

(9), (10): Recall that either (9) or (10) is satisfied strictly by  $p$ . In the case  $y - \bar{\beta}z < 0$ , i.e., (9) is satisfied strictly, we only need to check  $p_i^\epsilon$  satisfies (10):

$$\underline{\beta}z_i^\epsilon - y_i^\epsilon = \underline{\beta}((1 - \alpha_i^\epsilon) + \alpha_i^\epsilon z) - ((1 - \alpha_i^\epsilon)\bar{\beta} + \alpha_i^\epsilon y) = \alpha_i^\epsilon(\underline{\beta}z - y) \leq 0.$$

On the other hand, if  $\beta z - y < 0$ , i.e., (10) is satisfied strictly, then

$$y_i^\epsilon - \bar{\beta}z_i^\epsilon = \bar{\beta}(1 - \alpha_i^\epsilon) + \alpha_i^\epsilon y - \bar{\beta}((1 - \alpha_i^\epsilon) + \alpha_i^\epsilon z) = \alpha_i^\epsilon(y - \bar{\beta}z) \leq 0.$$

(12): Easily checked directly.

(13): Shown directly by

$$u_i^\epsilon - \underline{\gamma}x_i^\epsilon = \alpha_i^\epsilon(u - \underline{\gamma}x) \leq \alpha_i^\epsilon(t - \underline{\gamma}) = t_i^\epsilon - (1 - \alpha_i^\epsilon)\underline{\gamma} - \alpha_i^\epsilon\underline{\gamma} = t_i^\epsilon - \underline{\gamma}.$$

(15): Shown directly by

$$\begin{aligned} (u_i^\epsilon - \underline{\beta}x_i^\epsilon)(u_i^\epsilon - \underline{\gamma}x_i^\epsilon) &= (\alpha_i^\epsilon)^2(u - \underline{\beta}x)(u - \underline{\gamma}x) \\ &\leq (\alpha_i^\epsilon)^2(-\underline{\beta})x(t - \underline{\gamma}) = -\underline{\beta}(x_i^\epsilon\alpha_i^\epsilon(t - \underline{\gamma})) = -\underline{\beta}x_i^\epsilon(t_i^\epsilon - \underline{\gamma}). \end{aligned}$$

**Case (b):**  $z + x < 1$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon := \alpha_i^\epsilon x, \quad u_i^\epsilon := \alpha_i^\epsilon u, \quad y_i^\epsilon := \alpha_i^\epsilon y, \quad z_i^\epsilon := \alpha_i^\epsilon z, \quad t_i^\epsilon := (1 - \alpha_i^\epsilon)\underline{\gamma} + \alpha_i^\epsilon t.$$

It is clear that (7) and (9)–(12) are satisfied by  $p_i^\epsilon$  for  $i = 1, 2$ . By the assumption of this case (8) is strictly satisfied by  $p$ . The remaining inequalities (13) and (15) depend only on the variables  $x$ ,  $u$ , and  $t$ , and the definitions of  $u_i^\epsilon, x_i^\epsilon$ , and  $t_i^\epsilon$  are the same as in Case (a).

**Case (c):**  $y + u = 0$ ,  $z + x = 1$ , and  $y - \bar{\beta}z < 0$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon := \alpha_i^\epsilon x, \quad u_i^\epsilon := \alpha_i^\epsilon u, \quad y_i^\epsilon := \alpha_i^\epsilon y, \quad z_i^\epsilon := (1 - \alpha_i^\epsilon) + \alpha_i^\epsilon z, \quad t_i^\epsilon := (1 - \alpha_i^\epsilon)\underline{\gamma} + \alpha_i^\epsilon t.$$

(7), (8): Easily checked directly.

(9): Satisfied strictly by  $p$  by the assumption of this case.

(10): We show that (10) is satisfied strictly by  $p$ . Indeed, if  $\underline{\beta}z - y = 0$ , then the other equations for this case imply that  $u - \underline{\beta}x = -\underline{\beta}$ . Then, evaluating  $p$  in the left-hand-side of (15) yields:

$$(u - \underline{\beta}x)(u - \underline{\gamma}x) = -\underline{\beta}(u - \underline{\gamma}x) > -\underline{\beta}(xt - \underline{\gamma}x) = -\underline{\beta}x(t - \underline{\gamma})$$

and so  $p$  violates (15).

(12): Easily checked directly.

(13), (15): As the definitions of  $x_i^\epsilon$ ,  $u_i^\epsilon$ , and  $t_i^\epsilon$  are the same as in Case (a), the arguments in that case imply  $p_i^\epsilon$  satisfies (13) and (15) for  $\epsilon \in (0, 1)$ .

**Case (d):**  $y + u = 0$ ,  $z + x = 1$ , and  $y - \bar{\beta}z = 0$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon := x - \delta_i, \quad u_i^\epsilon := u - \delta_i \bar{\beta}, \quad y_i^\epsilon := y + \delta_i \bar{\beta}, \quad z_i^\epsilon := z + \delta_i, \quad t_i^\epsilon := t - \delta_i(\bar{\beta} - \underline{\gamma}).$$

(7), (8), (9): Easily checked directly.

(10): (10) is satisfied strictly by  $p$  by the same argument as in the previous case.

(12): We show that  $\bar{\gamma}x - u > 0$ , i.e., (12) is satisfied strictly by  $p$ . Indeed, the three equations in this case imply that  $\bar{\beta}x - u = \bar{\beta}$ . Thus,

$$\bar{\gamma}x - u = \bar{\gamma}x - \bar{\beta}x + \bar{\beta} = \bar{\gamma}x + (1 - x)\bar{\beta} > 0.$$

(13): Shown directly by

$$\begin{aligned} u_i^\epsilon - \underline{\gamma}x_i^\epsilon &= u - \delta_i \bar{\beta} - \underline{\gamma}(x - \delta_i) = u - \underline{\gamma}x - \delta_i(\bar{\beta} - \underline{\gamma}) \\ (34) \qquad \qquad \qquad &\leq t - \underline{\gamma} - \delta_i(\bar{\beta} - \underline{\gamma}) = t_i - \underline{\gamma}. \end{aligned}$$

(15): As  $y = \bar{\beta}z$  and  $z > 0$ , this implies  $y > 0$  and in turn  $u < 0$ . Thus,  $u - \underline{\beta}x < -\underline{\beta}x$  and so, for  $\epsilon > 0$  small enough, also  $u_i^\epsilon - \underline{\beta}x_i^\epsilon < -\underline{\beta}x_i^\epsilon$ . Combining this with (34) yields

$$(u_i^\epsilon - \underline{\beta}x_i^\epsilon)(u_i^\epsilon - \underline{\gamma}x_i^\epsilon) \leq -\underline{\beta}x_i^\epsilon(t_i - \underline{\gamma}). \quad \square$$

**4.3. Proof of Theorem 8.** We now state and prove the two main lemmas that support the proof of Theorem 8.

LEMMA 16. *Suppose  $\underline{\gamma} < \bar{\gamma} < 0$  and  $\underline{\beta} < 0 < \bar{\beta}$ . Let  $p = (x, u, y, z, t) \in R^2$  with  $0 < x < 1$  and  $\underline{\gamma} < t < \bar{\gamma}$ . If  $u < xt$ , then  $p$  is not an extreme point of  $R^2$ .*

*Proof.* First, we show that  $p$  satisfies (22) with strict inequality. Observe that the inequality (26) is valid for any point in  $R^2$ . Thus,

$$\begin{aligned} (\bar{\gamma} - \underline{\gamma})y + \underline{\gamma}(\bar{\gamma}x - u) + \bar{\beta}(u - \underline{\gamma}x) &< (\bar{\gamma} - \underline{\gamma})y + \underline{\gamma}(\bar{\gamma}x - xt) + \bar{\beta}(xt - \underline{\gamma}x) \\ &= (\bar{\gamma} - \underline{\gamma})y + (\bar{\gamma} - t)x\underline{\gamma} + (t - \underline{\gamma})\bar{\beta}x \leq (t - \underline{\gamma})\bar{\beta}. \end{aligned}$$

When  $u < xt$ , the inequality (22) is satisfied with strict inequality, just as (15) is satisfied by strict inequality when  $u < xt$  and  $\bar{\gamma} > 0$ . As the substitution of (22) for (15) is the only difference between the sets  $R^2$  and  $R^1$ , the arguments of Lemma 14 apply directly to this case, and we can conclude that if  $u < xt$ ,  $0 < x < 1$ , and  $\underline{\gamma} < t < \bar{\gamma}$ , then  $p$  is not an extreme point of  $R^2$ .  $\square$



LEMMA 17. Suppose  $\underline{\gamma} < \bar{\gamma} < 0$  and  $\underline{\beta} < 0 < \bar{\beta}$ . Let  $p = (x, u, y, z, t) \in R^2$  with  $0 < x < 1$  and  $\underline{\gamma} < t < \bar{\gamma}$ . If  $u > xt$ , then  $p$  is not an extreme point of  $R^2$ .

*Proof.* This proof has the same structure as the proof of Lemma 14. First, by Proposition 12,  $u > xt$  implies that  $p$  satisfies (11) and (14) with strict inequality, and by Proposition 13 if also  $y > 0$ , then  $p$  satisfies (18) with strict inequality. Also, as  $\bar{\gamma} < 0$ , it follows from  $u \leq \bar{\gamma}x$  and  $x > 0$  that  $u < 0$ . It remains to show that the points  $p_i^\epsilon$  are feasible for the inequalities (7)–(10), (12), (13), and (22). We consider four cases.

**Case (a):**  $y + u < 0$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$\begin{aligned} x_i^\epsilon &:= (1 - \alpha_i^\epsilon) + \alpha_i^\epsilon x, & u_i^\epsilon &:= \bar{\gamma}(1 - \alpha_i^\epsilon) + \alpha_i^\epsilon u, & y_i^\epsilon &:= \alpha_i^\epsilon y, \\ z_i^\epsilon &:= \alpha_i^\epsilon z, & t_i^\epsilon &:= (1 - \alpha_i^\epsilon)\bar{\gamma} + \alpha_i^\epsilon t. \end{aligned}$$

(7): Satisfied strictly by  $p$  by the assumption of this case.

(8)–(10): Easily checked directly.

(12): Shown directly by

$$(35) \quad \bar{\gamma}x_i^\epsilon - u_i^\epsilon = \bar{\gamma}(1 - \alpha_i^\epsilon) + \bar{\gamma}\alpha_i^\epsilon x - (1 - \alpha_i^\epsilon)\bar{\gamma} - \alpha_i^\epsilon u = \alpha_i^\epsilon(\bar{\gamma}x - u) \geq 0.$$

(13): Shown directly by

$$\begin{aligned} (36) \quad u_i^\epsilon - \underline{\gamma}x_i^\epsilon &= \bar{\gamma}(1 - \alpha_i^\epsilon) + \alpha_i^\epsilon u - \underline{\gamma}(1 - \alpha_i^\epsilon) - \underline{\gamma}\alpha_i^\epsilon x \\ &= (\bar{\gamma} - \underline{\gamma})(1 - \alpha_i^\epsilon) + \alpha_i^\epsilon(u - \underline{\gamma}x) \\ &\leq (\bar{\gamma} - \underline{\gamma})(1 - \alpha_i^\epsilon) + \alpha_i^\epsilon(t - \underline{\gamma}) \\ (37) \quad &= (\bar{\gamma} - \underline{\gamma})(1 - \alpha_i^\epsilon) + t_i^\epsilon - (1 - \alpha_i^\epsilon)\bar{\gamma} - \alpha_i^\epsilon \underline{\gamma} = t_i^\epsilon - \underline{\gamma}. \end{aligned}$$

(22): Using (35) and (36), we get

$$\begin{aligned} &(\bar{\gamma} - \underline{\gamma})y_i^\epsilon + \underline{\gamma}(\bar{\gamma}x_i^\epsilon - u_i^\epsilon) + \bar{\beta}(u_i^\epsilon - \underline{\gamma}x_i^\epsilon) \\ &= \alpha_i^\epsilon \left( (\bar{\gamma} - \underline{\gamma})y + \underline{\gamma}(\bar{\gamma}x - u) + \bar{\beta}(u - \underline{\gamma}x) \right) + \bar{\beta}(\bar{\gamma} - \underline{\gamma})(1 - \alpha_i^\epsilon) \\ &\leq \alpha_i^\epsilon \bar{\beta}(t - \underline{\gamma}) + (1 - \alpha_i^\epsilon)\bar{\beta}(\bar{\gamma} - \underline{\gamma}) = \bar{\beta}(t_i^\epsilon - \underline{\gamma}) \end{aligned}$$

where the last equation follows from (37).

**Case (b):**  $z + x < 1$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon := \alpha_i^\epsilon x, \quad u_i^\epsilon := \alpha_i^\epsilon u, \quad y_i^\epsilon := \alpha_i^\epsilon y, \quad z_i^\epsilon := \alpha_i^\epsilon z, \quad t_i^\epsilon := \alpha_i^\epsilon t + (1 - \alpha_i^\epsilon)\underline{\gamma}.$$

(7): Easily checked directly.

(8): Satisfied strictly by  $p$  by the assumption of this case.

(9), (10), (12): Easily checked directly.

(13): Shown directly by

$$(38) \quad \begin{aligned} u_i^\epsilon - \underline{\gamma}x_i^\epsilon &= \alpha_i^\epsilon u - \underline{\gamma}\alpha_i^\epsilon x \leq \alpha_i^\epsilon(t - \underline{\gamma}) = t_i^\epsilon - (1 - \alpha_i^\epsilon)\underline{\gamma} - \alpha_i^\epsilon \underline{\gamma} \\ &= t_i^\epsilon - \underline{\gamma}. \end{aligned}$$

(22): Shown directly by

$$\begin{aligned} &(\bar{\gamma} - \underline{\gamma})y_i^\epsilon + \underline{\gamma}(\bar{\gamma}x_i^\epsilon - u_i^\epsilon) + \bar{\beta}(u_i^\epsilon - \underline{\gamma}x_i^\epsilon) \\ &= \alpha_i^\epsilon \left( (\bar{\gamma} - \underline{\gamma})y + \underline{\gamma}(\bar{\gamma}x - u) + \bar{\beta}(u - \underline{\gamma}x) \right) \leq \alpha_i^\epsilon \bar{\beta}(t - \underline{\gamma}) = \bar{\beta}(t_i^\epsilon - \underline{\gamma}) \end{aligned}$$

where the last equation follows as in (38).

**Case (c):**  $y - \bar{\beta}z < 0$  and  $\underline{\beta}z - y < 0$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon := \alpha_i^\epsilon x, \quad u_i^\epsilon := \alpha_i^\epsilon u, \quad y_i^\epsilon := \alpha_i^\epsilon y, \quad z_i^\epsilon := (1 - \alpha_i^\epsilon) + \alpha_i^\epsilon z, \quad t_i^\epsilon := \alpha_i^\epsilon t + (1 - \alpha_i^\epsilon)\underline{\gamma}.$$

Then, it is easily seen by construction that  $p_i^\epsilon$  satisfies (8) for any  $\epsilon \in (0, 1)$ ,  $i = 1, 2$ . As the definitions of  $x_i^\epsilon$ ,  $u_i^\epsilon$ ,  $y_i^\epsilon$ , and  $t_i^\epsilon$  are the same as in Case (b), the arguments of Case (b) apply for all inequalities that do not contain the variable  $z$ . This just leaves and (9) and (10), which by assumption are satisfied strictly by  $p$ , and so the proof for this case is complete.

**Case (d):**  $y + u = 0$ ,  $z + x = 1$ , and either  $y - \bar{\beta}z = 0$  or  $\underline{\beta}z - y = 0$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon := (1 - \alpha_i^\epsilon) + \alpha_i^\epsilon x, \quad u_i^\epsilon := \alpha_i^\epsilon u, \quad y_i^\epsilon := \alpha_i^\epsilon y, \quad z_i^\epsilon := \alpha_i^\epsilon z, \quad t_i^\epsilon := (1 - \alpha_i^\epsilon)\frac{\underline{\gamma}\bar{\gamma}}{\beta} + \alpha_i^\epsilon t.$$

(7)–(10): Easily checked directly.

(12): We show that  $p$  satisfies (12) strictly. Suppose for purpose of contradiction that  $\bar{\gamma}x - u = 0$ . Then,

$$\begin{aligned} (\bar{\gamma} - \underline{\gamma})y + \underline{\gamma}(\bar{\gamma}x - u) + \bar{\beta}(u - \underline{\gamma}x) &= (\bar{\gamma} - \underline{\gamma})y + \bar{\beta}(\bar{\gamma}x - \underline{\gamma}x) \\ &= (\bar{\gamma} - \underline{\gamma})(y + \bar{\beta}x) = (\bar{\gamma} - \underline{\gamma})\bar{\beta} > \bar{\beta}(t - \underline{\gamma}) \end{aligned}$$

where we have used  $y + \bar{\beta}x = \bar{\beta}z + \bar{\beta}x = \bar{\beta}$ . Thus, when  $\bar{\gamma}x - u = 0$  then (22) is violated, and hence we conclude that (12) is satisfied strictly by  $p$ .

(13): We show that  $p$  satisfies (13) strictly. Indeed, as  $y = -u$ , we find that

$$(\bar{\gamma} - \underline{\gamma})y + \underline{\gamma}(\bar{\gamma}x - u) = (\bar{\gamma} - \underline{\gamma})(-u) + \underline{\gamma}(\bar{\gamma}x - u) = \bar{\gamma}(\underline{\gamma}x - u) > 0$$

since  $\bar{\gamma} < 0$  and  $\underline{\gamma}x - u < 0$ . Thus, rearranging inequality (22) yields

$$u - \underline{\gamma}x \leq t - \underline{\gamma} - \frac{1}{\bar{\beta}}((\bar{\gamma} - \underline{\gamma})y + \underline{\gamma}(\bar{\gamma}x - u)) < t - \underline{\gamma}$$

which shows (13) is satisfied strictly by  $p$ .

(22): Shown directly by

$$\begin{aligned} &(\bar{\gamma} - \underline{\gamma})y_i^\epsilon + \underline{\gamma}(\bar{\gamma}x_i^\epsilon - u_i^\epsilon) + \bar{\beta}(u_i^\epsilon - \underline{\gamma}x_i^\epsilon) \\ &= \alpha_i^\epsilon((\bar{\gamma} - \underline{\gamma})y + \underline{\gamma}(\bar{\gamma}x - u) + \bar{\beta}(u - \underline{\gamma}x)) + \underline{\gamma}\bar{\gamma}(1 - \alpha_i^\epsilon) - \bar{\beta}\underline{\gamma}(1 - \alpha_i^\epsilon) \\ &\leq \alpha_i^\epsilon\bar{\beta}(t - \underline{\gamma}) - (1 - \alpha_i^\epsilon)\underline{\gamma}(\bar{\beta} - \bar{\gamma}) \\ &= \bar{\beta}\left(t_i^\epsilon - (1 - \alpha_i^\epsilon)\frac{\underline{\gamma}\bar{\gamma}}{\beta} - \underline{\gamma}\alpha_i^\epsilon\right) - (1 - \alpha_i^\epsilon)\underline{\gamma}(\bar{\beta} - \bar{\gamma}) \\ &= \bar{\beta}(t_i^\epsilon - \underline{\gamma}) - (1 - \alpha_i^\epsilon)(\underline{\gamma}\bar{\gamma}) + (1 - \alpha_i^\epsilon)(\underline{\gamma}\bar{\gamma}) = \bar{\beta}(t_i^\epsilon - \underline{\gamma}). \quad \square \end{aligned}$$

**4.4. Proof of Theorem 9.** We now state and prove the two main lemmas that support the proof of Theorem 9. We prepare the proofs with the following proposition.

PROPOSITION 18. *Let  $\underline{\beta} < 0$ . If  $p \in \mathbb{R}^3$ , then  $p$  satisfies the following inequality:*

$$(39) \quad (\underline{\gamma} - \underline{\beta})x \leq -\underline{\beta}$$

*In addition, if  $p$  satisfies (7), (8), (10), and (11) at equality, then it satisfies (39) at equality.*

*Proof.* First, aggregating (7) with weight 1, (8) with weight  $-\underline{\beta}$ , (10) with weight 1, and (11) with weight  $-1$ , yields (39). If (7), (8), (10), and (11) are all satisfied at equality, then  $p$  satisfies (39) at equality.  $\square$

LEMMA 19. *Suppose  $0 < \underline{\gamma} < \bar{\gamma}$  and  $\underline{\beta} < 0 < \bar{\beta}$ . Let  $p = (x, u, y, z, t) \in R^3$  with  $0 < x < 1$  and  $\underline{\gamma} < t < \bar{\gamma}$ . If  $u < xt$ , then  $p$  is not an extreme point of  $R^3$ .*

*Proof.* This proof has the same structure as the proof of Lemma 14. By Proposition 12,  $p$  satisfies (12), (13), and (15) with strict inequality. Also, as  $u \geq \underline{\gamma}x > 0$ , (7) implies that  $y < 0 \leq \bar{\beta}z$ , and hence  $p$  satisfies (9) with strict inequality. In addition, by (28),

$$\bar{\gamma}x - u \leq \frac{-\underline{\beta}}{\underline{\gamma} - \underline{\beta}}(\bar{\gamma} - t) < \bar{\gamma} - t$$

as  $\bar{\gamma} - t > 0$  and  $\underline{\gamma} - \underline{\beta} > -\underline{\beta}$  because  $\underline{\gamma} > 0$ , and so  $p$  satisfies (14) with strict inequality. It remains to show that the points  $p_i^\epsilon$  satisfy (7), (8), (10), (11), and (28) for  $\epsilon$  small enough. We consider four cases.

**Case (a):**  $y + u < 0$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$\begin{aligned} x_i^\epsilon &:= \alpha_i^\epsilon x, & u_i^\epsilon &:= \alpha_i^\epsilon u, & y_i^\epsilon &:= (1 - \alpha_i^\epsilon)\underline{\beta} + \alpha_i^\epsilon y, \\ z_i^\epsilon &:= (1 - \alpha_i^\epsilon) + \alpha_i^\epsilon z, & t_i^\epsilon &:= (1 - \alpha_i^\epsilon)\bar{\gamma} + \alpha_i^\epsilon t. \end{aligned}$$

(7): Satisfied strictly by  $p$  by the assumption of this case.

(8), (10), (11): Easily checked directly.

(28): Shown directly by

$$\begin{aligned} (\underline{\gamma} - \underline{\beta})(\bar{\gamma}x_i^\epsilon - u_i^\epsilon) &= \alpha_i^\epsilon(\underline{\gamma} - \underline{\beta})(\bar{\gamma}x - u) \\ &\leq \alpha_i^\epsilon(-\underline{\beta})(\bar{\gamma} - t) = -\underline{\beta}(\alpha_i^\epsilon\bar{\gamma} - t_i^\epsilon + (1 - \alpha_i^\epsilon)\bar{\gamma}) = -\underline{\beta}(\bar{\gamma} - t_i^\epsilon). \end{aligned}$$

**Case (b):**  $z + x < 1$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon := \alpha_i^\epsilon x, \quad u_i^\epsilon := \alpha_i^\epsilon u, \quad y_i^\epsilon := \alpha_i^\epsilon y, \quad z_i^\epsilon := \alpha_i^\epsilon z, \quad t_i^\epsilon := (1 - \alpha_i^\epsilon)\bar{\gamma} + \alpha_i^\epsilon t.$$

Then,  $p_i^\epsilon$  is easily seen to satisfy (7), (10), and (11) for any  $\epsilon \in (0, 1)$ . (8) is satisfied strictly by the assumption of this case. In addition, as the definitions of  $u_i^\epsilon$ ,  $x_i^\epsilon$ , and  $t_i^\epsilon$  are the same as in Case (a), (28) is satisfied by  $p_i^\epsilon$  for  $i = 1, 2$  and any  $\epsilon \in (0, 1)$ .

**Case (c):**  $y > \underline{\beta}z$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon := \alpha_i^\epsilon x, \quad u_i^\epsilon := \alpha_i^\epsilon u, \quad y_i^\epsilon := \alpha_i^\epsilon y, \quad z_i^\epsilon := (1 - \alpha_i^\epsilon) + \alpha_i^\epsilon z, \quad t_i^\epsilon := (1 - \alpha_i^\epsilon)\bar{\gamma} + \alpha_i^\epsilon t.$$

Then,  $p_i^\epsilon$  is easily seen to satisfy (7), (8), and (11) for any  $\epsilon \in (0, 1)$ . (10) is satisfied strictly by the assumption of this case. In addition, as the definitions of  $u_i^\epsilon$ ,  $x_i^\epsilon$ , and  $t_i^\epsilon$  are the same as in Case (a), (28) is satisfied by  $p_i^\epsilon$  for  $i = 1, 2$  and any  $\epsilon \in (0, 1)$ .

**Case (d):**  $y + u = 0$ ,  $z + x = 1$ , and  $y = \underline{\beta}z$ . For  $\epsilon > 0$ , define  $p_i^\epsilon = (x_i^\epsilon, u_i^\epsilon, y_i^\epsilon, z_i^\epsilon, t_i^\epsilon)$  where, for  $i = 1, 2$ ,

$$x_i^\epsilon := x - \delta_i^\epsilon, \quad u_i^\epsilon := u - \underline{\beta}\delta_i^\epsilon, \quad y_i^\epsilon := y + \underline{\beta}\delta_i^\epsilon, \quad z_i^\epsilon := z + \delta_i^\epsilon, \quad t_i^\epsilon := t + \delta_i^\epsilon \frac{(\underline{\gamma} - \underline{\beta})(\bar{\gamma} - \underline{\beta})}{(-\underline{\beta})}.$$

(7), (8), (10): Easily checked directly.

(11): We show that (11) is satisfied strictly by  $p$ . Indeed, suppose to the contrary that  $\underline{\gamma}x - u = 0$ . Then, by Proposition 18,  $(\underline{\gamma} - \underline{\beta})x = -\underline{\beta}$ . Thus, using  $u < xt$ ,  $\underline{\gamma} > 0$  and  $-\underline{\beta} > 0$ ,

$$(\underline{\gamma} - \underline{\beta})(\bar{\gamma}x - u) > (\underline{\gamma} - \underline{\beta})(\bar{\gamma}x - xt) = -\underline{\beta}(\bar{\gamma} - t)$$

and hence (28) is violated. Thus, (11) is satisfied strictly by  $p$ .

(28): Since  $u > xt$  and Proposition 18 we show the validity of (28) by

$$\begin{aligned}
(\underline{\gamma} - \underline{\beta})(\bar{\gamma}x_i^\epsilon - u_i^\epsilon) &= (\underline{\gamma} - \underline{\beta})(\bar{\gamma}(x - \delta_i) - (u - \beta\delta_i)) \\
&= (\underline{\gamma} - \underline{\beta})(\bar{\gamma}x - u) - \delta_i(\underline{\gamma} - \underline{\beta})(\bar{\gamma} - \underline{\beta}) \\
&< (\underline{\gamma} - \underline{\beta})x(\bar{\gamma} - t) - \delta_i(\underline{\gamma} - \underline{\beta})(\bar{\gamma} - \underline{\beta}) \\
&\leq -\underline{\beta}(\bar{\gamma} - t) - \delta_i(\underline{\gamma} - \underline{\beta})(\bar{\gamma} - \underline{\beta}) \\
&= -\underline{\beta}\left(\bar{\gamma} - t_i + \delta_i\frac{(\underline{\gamma} - \underline{\beta})(\bar{\gamma} - \underline{\beta})}{(-\underline{\beta})}\right) - \delta_i(\underline{\gamma} - \underline{\beta})(\bar{\gamma} - \underline{\beta}) \\
&= -\underline{\beta}(\bar{\gamma} - t_i). \quad \square
\end{aligned}$$

LEMMA 20. Suppose  $0 < \underline{\gamma} < \bar{\gamma}$  and  $\underline{\beta} < 0 < \bar{\beta}$ . Let  $p = (x, u, y, z, t) \in R^3$  with  $0 < x < 1$  and  $\underline{\gamma} < t < \bar{\gamma}$ . If  $u > xt$ , then  $p$  is not an extreme point of  $R^3$ .

*Proof.* Using  $\underline{\gamma} - \underline{\beta} > 0$ , we have

$$(\underline{\gamma} - \underline{\beta})(x\bar{\gamma} - u) < (\underline{\gamma} - \underline{\beta})x(\bar{\gamma} - t) \leq -\underline{\beta}(\bar{\gamma} - t)$$

by (39) in Proposition 18.

When  $u > xt$ , the inequality (28) is satisfied with strict inequality, just as (18) is satisfied by strict inequality when  $u > xt$  and  $\underline{\gamma} < 0$  as in Case 1. As the substitution of (28) for (18) is the only difference between the sets  $R^3$  and  $R^1$ , Lemma 15 applies directly to this case, and we can conclude that if  $u > xt$ ,  $0 < x < 1$ , and  $\underline{\gamma} < t < \bar{\gamma}$ , then  $p$  is not an extreme point of  $R^3$ .  $\square$

**5. Computational Results.** In this section, we present results from computational experiments conducted on instances from the literature and on larger randomly generated instances derived from the instances in the literature. We show that the proposed inequalities indeed strengthen the relaxation of the  $pq$ -formulation and are able to speed up the global solution process, especially on sparse instances.

**5.1. Computational setup.** The experiments were conducted on a cluster with 64bit Intel Xeon X5672 CPUs at 3.2 GHz with 12 MB cache and 48 MB main memory. To limit the impact of variability in machine performance, e.g., by cache misses, we run only one job on each node at a time.

The model is implemented in the GAMS language and processed with GAMS version 24.7.1. The  $pq$ -formulation is solved to global optimality with SCIP version 3.2 which used CPLEX 12.6.3 as LP solver and Ipopt 3.12 as local NLP solver. The relaxations, which are LPs or SOCPs, are solved with CPLEX 12.6.3. We used the predefined timelimit of 1000 seconds and use a relative gap of  $10^{-6}$  as termination criterion (GAMS options OPTCA = 0.0 and OPTCR =  $10^{-6}$ ).

**5.2. Adding the inequalities.** Recall that the initial step to construct the 5-variable relaxation was to focus on a (Attribute, Pool, Output) tuple and extend the model by the aggregated variables  $u, x, z, y, t$  for each such pair. We follow this approach in the implementation. We extend the model by the aggregated variables and rely on the solver to replace or disaggregate the variables in the constraints if it is considered advantageous. We add the linear inequalities whenever they are valid (specifically (22) is added whenever  $\bar{\beta} > 0$  and (28) is added whenever  $\underline{\beta} < 0$ ). Inequality (15) is second-order cone (SOC) representable and could in principle be added directly as SOC constraint. However, we are not able to directly formulate

(18) using a linear or second-order cone representation and we thus resort to a cutting plane algorithm. Namely, whenever the relaxation solution has  $y > 0$  for a specific (Attribute, Pool, Output), a gradient inequality at this point is separated and the relaxation is solved again. Note that the gradient inequality is also valid for  $y \leq 0$  due to Lemma 4. Since the gradient inequalities towards the end of the separation loop become almost parallel, the interior point SOCP solver frequently runs into numerical trouble. To circumvent this, (15) is not added directly to the model, but linear gradient inequalities are also separated from all conic inequalities in the same separation loop. The major advantage is that all relaxations are then LPs and thus solved very efficiently. This approach in our experience provides much better running times than solving SOCP relaxations in the separation loop.

We separate the inequalities only at the root node of the spatial branch-and-bound algorithm. More precisely, we set up the separation loop for both inequalities and separate until the absolute violation of the conic inequality and inequality (18) are below  $10^{-4}$  and  $10^{-5}$ , respectively. Then we pass the  $pq$ -formulation and all inequalities that have been separated to SCIP and solve the problem globally. The separation therefore does not make use of any model changes or strengthening that SCIP performs during preprocessing or from propagations during its own cutting plane loop.

In the following we use  $pq$ -relaxation to refer to the McCormick relaxation of the  $pq$ -formulation. The relaxation that arises by strengthening the  $pq$ -relaxation with our valid inequalities is called  $pq^+$ -relaxation.

**5.3. Instances.** We perform experiments on two sets of instances: The pooling instances from the GAMS LIB [16] and new instances that we randomly generated based on structures from the GAMS LIB instances. The GAMS LIB instances are encoded in the `pool` model as different cases yielding 14 instances. All of them were first presented in scientific publications about the pooling problem. It comprises three instances on the original network from Haverly [21, 22]. Furthermore, it contains instances from the publications [15, 8, 1, 4].

The random instances are generated in the following way. The basis are copies of the Haverly instances. The resulting disconnected graphs are then supplemented by randomly adding a specific number of admissible edges in a pooling network. As the resulting network might still be disconnected, the first edges are chosen as to connect two disconnected components until the graph is connected. As the GAMS LIB includes three instances of the Haverly network with different parameters, the distribution among the three Haverly instances is sampled randomly. Next, for each copy a factor  $\phi \in [0.5, 2]$  is sampled uniformly and all concentration parameters, i.e.,  $\lambda_{ik}$  and  $\bar{\mu}_{jk}$  of that copy are scaled by  $\phi$ . Lower bounds on the concentration are not used in these instances but could be sampled and handled in the separation in a similar way.

We generated instances with 10, 15, and 20 copies of the Haverly network. The number of edges to be added are multiples of the number of copies of the Haverly network. For each such pair of number of copies and number of additional edges, we sample 10 instances. In total 180 instances are generated.

The new instances and the scripts to create them are available online<sup>1</sup>.

**5.4. Results.** First, we consider the 14 GAMS LIB instances. For six instances the  $pq$ -relaxation provides the optimal bound and hence these instances are not considered anymore. Table 2 shows results on the remaining eight GAMS LIB instances.

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<sup>1</sup><https://github.com/poolinginstances/poolinginstances>, commit e50a2c31ceed

Instance	Graph		$pq$		$pq^+$			Opt
	Nodes	Arcs	Absolute	Gap	Absolute	Gap	Closed	
adhya1	11	13	-766.3	39.4 %	-697.0	26.8 %	32.0 %	-549.8
adhya2	11	13	-570.8	3.8 %	-568.3	3.4 %	11.8 %	-549.8
adhya3	15	20	-571.3	1.8 %	-570.7	1.7 %	6.3 %	-561.0
adhya4	15	18	-961.2	9.5 %	-955.4	8.9 %	7.0 %	-877.6
bental4	7	4	-550.0	22.2 %	-450.0	0.0 %	100.0 %	-450.0
haverly1	6	6	-500.0	25.0 %	-400.0	0.0 %	100.0 %	-400.0
haverly2	6	6	-1000.0	66.7 %	-600.0	0.0 %	100.0 %	-600.0
haverly3	6	6	-800.0	6.7 %	-791.7	5.6 %	16.7 %	-750.0

TABLE 2

Results on GAMS LIB instances where the  $pq$ -formulation does not provide the optimum

Cop.	Graph			Gap [%]		Global $pq$			Global $pq^+$		
	$ V $	$ A $	$ A^+ $	$pq$	$pq^+$	TL	Time	Nodes	TL	Time	Nodes
10	60	70	10	13.0	3.2	0	5.0	7098.1	0	1.8	213.9
	60	80	20	8.3	3.8	0	3.4	3011.6	0	3.4	727.0
	60	90	30	4.7	2.9	0	3.1	1397.2	0	3.2	371.4
	60	100	40	3.0	1.9	0	2.3	993.2	0	4.1	530.4
	60	110	50	2.6	2.1	0	3.3	1034.4	0	6.0	665.9
	60	120	60	3.3	2.4	0	6.3	2320.4	0	9.3	1511.6
15	90	105	15	10.6	3.2	0	63.0	106880.6	0	7.0	2023.2
	90	120	30	7.2	3.3	1	53.2	40031.5	1	20.0	3480.5
	90	135	45	4.9	3.4	1	36.6	24087.1	0	31.0	8202.0
	90	150	60	4.1	3.0	1	33.4	19234.3	0	24.0	5043.2
	90	165	75	3.3	2.5	0	21.2	13919.3	0	37.1	10576.1
	90	180	90	3.8	3.0	1	47.4	21998.2	1	51.8	8300.6
20	120	140	20	13.4	4.3	9	993.9	1655439.0	1	44.3	7327.0
	120	160	40	6.0	2.9	4	296.9	175642.9	3	116.8	18319.4
	120	180	60	4.5	2.8	5	287.6	84123.7	4	213.3	29497.7
	120	200	80	4.1	2.8	2	84.3	40476.0	2	68.5	12186.5
	120	220	100	3.1	2.3	3	159.1	44945.7	3	142.3	20325.7
	120	240	120	2.5	2.0	2	187.5	69610.8	3	224.1	36090.3
Total	-	-	-	5.7	2.9	29	37.1	12685.7	18	25.0	3108.0

TABLE 3

Results on randomly generated instances

Along with the size of the graph in terms of number of nodes and arcs, Table 2 presents the value of the different relaxations and their gaps. The column “Opt” shows the global optimum computed by solving the nonconvex  $pq$ -formulation. The instances are small, but the results are encouraging. Our relaxation gives a stronger dual bound on all instances compared to the  $pq$ -relaxation and on three instances the gap is closed completely.

Table 3 presents results on the larger randomly generated networks. The instances are grouped by the number of copies of the Haverly network (first column) and by the number of edges that have been added to the network (column  $|A^+|$ ). Each row thus provides aggregated results over 10 instances. The last row represents the total

over all instances. The group of columns labeled with “Graph” shows statistics about the graphs. Besides the number of random arcs added  $|A^+|$ , the number of nodes  $|V|$  and arcs  $|A|$  is shown. The numbers are identical within each group of instances. Next, the average gap for the  $pq$ -relaxation and the  $pq^+$ -relaxation is shown. For both approaches the gap is computed w.r.t. the best known primal bound for the problem and thus reflects only differences in the dual bound. Finally, the last two groups of columns show statistics about the global solution process using the  $pq$ -formulation and  $pq^+$ -relaxation at the root. We report number of instances that were terminated due to the time limit (column “TL”), time, and number of nodes. For time and nodes, the shifted geometric mean with shift 2 and 100, respectively, is used to aggregate the results. Furthermore, only instances where both approaches finished within the time limit are considered in the computation of the number of nodes. For  $pq^+$ , the separation time for the nonlinear inequalities is taken into account by adding it to the time SCIP needed to solve the problem.

The  $pq^+$ -relaxation is effective in reducing the root gap, leaving an average gap of 2.9% compared to the 5.7% of the  $pq$ -relaxation. The  $pq^+$ -relaxation performs especially well on instances with sparse networks. This is expected, since the relaxation provides the optimal dual bound on two of the three Haverly instances (see Table 2) that we used to construct the random instances. All but one instance of the testset experience an improvement of the dual bounds due to the additional inequalities. The most notable effect of the stronger root bound is on the number of branch&bound nodes needed to solve an instances to global optimality. The shifted geometric mean of the nodes is reduced from 12685 to 3108, a reduction of 75% over the full set of instances. While reductions are stronger on sparse instances, significant reductions are observed among all classes of instances. In terms of time to optimality, the stronger relaxation pays off only for sparse instances. As the instances become denser, the  $pq$ -formulation achieves better running times in the shifted geometric mean. Over all instances, however, the shifted geometric mean is reduced from 37.1 to 25.0 seconds. A significant portion of this improvement comes from instances with 20 Haverly networks and only 20 additional edges. From the 10 instances of this class, only one instance is solved within the time limit (in 940 seconds) by the  $pq$ -formulation while all but one are solved using the  $pq^+$ -relaxation. The dual bound is exactly the problem for the  $pq$ -formulation on these instances. The approach with the  $pq$ -formulation found an optimal solution always within the first 184 seconds of the optimization and then used a massive amount of branching nodes to close the gap. Overall,  $pq^+$  solves 11 instances more within the timelimit than the  $pq$ -formulation.

**6. Conclusions.** We have derived new valid inequalities for the pooling problem by studying a set defined by a single product, a single pool, and a single attribute, and performing a variable aggregation. Since we have also shown these inequalities define the convex hull in many cases, further improvements to the relaxation of the pooling problem will need to consider more aspects of the problem. For example, still with a fixed attribute  $k$ , output  $j$ , and pool  $\ell$ , one may consider studying valid inequalities for a set in which the variables  $x_{ij}$ ,  $w_{i\ell j}$ , and  $q_{i\ell}$ , for  $i \in I$  are included, rather than being summarized in the variables  $z_{i\ell}$ ,  $t_{k\ell}$  and  $u_{k\ell j}$ . Alternatively, one may still use these summary variables, but study a set that includes multiple pools. The latter approach may yield further improved relaxations, since it avoids the need to treat all flows to the fixed product that pass through pools other than the fixed pool as by-pass flows.

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#### REFERENCES

- [1] N. ADHYA, M. TAWARMALANI, AND N. V. SAHINIDIS, *A lagrangian approach to the pooling problem*, *Industrial & Engineering Chemistry Research*, 38 (1999), pp. 1956–1972.
- [2] F. A. AL-KHAYYAL AND J. E. FALK, *Jointly constrained biconvex programming*, *Mathematics of Operations Research*, 8 (1983), pp. 273–286.
- [3] M. ALFAKI AND D. HAUGLAND, *Strong formulation for the pooling problem*, *Journal of Global Optimization*, 56 (2013), pp. 897–916.
- [4] C. AUDET, J. BRIMBERG, P. HANSEN, S. L. DIGABEL, AND N. MLADENOVIC, *Pooling problem: Alternate formulations and solution methods*, *Management Science*, 50 (2004), pp. 761–776.
- [5] M. BAGAJEWICZ, *A review of recent design procedures for water networks in refineries and process plants*, *Computers & Chemical Engineering*, 24 (2000), pp. 2093 – 2113.
- [6] T. E. BAKER AND L. S. LASDON, *Successive linear programming at Exxon*, *Management Science*, 31 (1985), pp. 264–274.
- [7] R. BALTEAN-LUGOJAN AND R. MISENER, *Piecewise parametric structure in the pooling problem: from sparse strongly-polynomial solutions to NP-hardness*, *Journal of Global Optimization*, (2017), <https://doi.org/10.1007/s10898-017-0577-y>.
- [8] A. BEN-TAL, G. EIGER, AND V. GERSHOVITZ, *Global minimization by reducing the duality gap*, *Mathematical Programming*, 63 (1994), pp. 193–212.
- [9] N. BOLAND, T. KALINOWSKI, AND F. RIGTERINK, *A polynomially solvable case of the pooling problem*, *Journal of Global Optimization*, 67 (2017), pp. 621–630.
- [10] F. CECCON, G. KOUYIALIS, AND R. MISENER, *Using functional programming to recognize named structure in an optimization problem: Application to pooling*, *AIChE Journal*, (2016).
- [11] C. D’AMBROSIO, J. T. LINDEROTH, AND J. LUEDTKE, *Valid inequalities for the pooling problem with binary variables*, in *Integer Programming and Combinatorial Optimization*, 15th International IPCO Conference Proceedings, Springer, 2011, pp. 117–129.
- [12] C. W. DEWITT, L. S. LASDON, A. D. WARREN, D. A. BRENNER, AND S. A. MELHEM, *OMEGA: An Improved Gasoline Blending System for Texaco*, *Interfaces*, 19 (1989), pp. 85–101.
- [13] S. S. DEY AND A. GUPTE, *Analysis of MILP techniques for the pooling problem*, *Operations Research*, 63 (2015), pp. 412–427.
- [14] C. A. FLOUDAS AND A. AGGARWAL, *A decomposition strategy for global optimum search in the pooling problem*, *ORSA Journal on Computing*, 2 (1990), pp. 225–235.
- [15] L. FOULDS, D. HAUGLAND, AND K. JORNSTEN, *A bilinear approach to the pooling problem*, *Optimization*, 24 (1992), pp. 165–180.
- [16] GAMS MODEL LIBRARY, <http://www.gams.com/modlib/modlib.htm>.
- [17] A. GUPTE, *Mixed Integer Bilinear Programming with Applications to the Pooling Problem*, PhD thesis, Georgia Institute of Technology, 2012.
- [18] A. GUPTE, S. AHMED, S. DEY, AND M. CHEON, *Pooling problems: an overview*, *Optimization and Analytics in the Oil and Gas Industry*, acceptor (2015).
- [19] A. GUPTE, S. AHMED, S. S. DEY, AND M. S. CHEON, *Relaxations and discretizations for the pooling problem*, *Journal of Global Optimization*, 67 (2017), pp. 631–669.
- [20] D. HAUGLAND, *The computational complexity of the pooling problem*, *Journal of Global Optimization*, 64 (2015), pp. 199–215.
- [21] C. A. HAVERLY, *Studies of the behavior of the recursion for the pooling problem*, *SIGMAP Bulletin*, 25 (1978), pp. 19–28.
- [22] C. A. HAVERLY, *Behaviour of the recursion model - more studies*, *SIGMAP Bulletin*, 26 (1979), pp. 12–28.
- [23] J. KALLARATH, *Mixed integer optimization in the chemical process industry: Experience, potential and future perspectives*, *Chemical Engineering Research and Design*, 78 (2000), pp. 809–822.



- [24] J. LUEDTKE, C. D'AMBROSIO, J. LINDEROTH, AND J. SCHWEIGER, *Strong convex nonlinear relaxations of the pooling problem: Extreme points*, Tech. Report ZIB-Report 18-13, Zuse Institute Berlin, Takustr. 7, 14195 Berlin, March 2018.
- [25] G. P. MCCORMICK, *Computability of global solutions to factorable nonconvex programs: Part I—Convex underestimating problems*, Mathematical Programming, 10 (1976), pp. 147–175.
- [26] C. A. MEYER AND C. A. FLOUDAS, *Global optimization of a combinatorially complex generalized pooling problem*, AIChE Journal, 52 (2006), pp. 1027–1037.
- [27] R. MISENER AND C. FLOUDAS, *Advances for the pooling problem: Modeling, global optimization, & computational studies*, Applied and Computational Mathematics, 8 (2009), pp. 3–22.
- [28] R. MISENER AND C. A. FLOUDAS, *Global optimization of large-scale generalized pooling problems: Quadratically constrained minlp models*, Industrial & Engineering Chemistry Research, 49 (2010), pp. 5424–5438.
- [29] R. MISENER, C. E. GOUNARIS, AND C. A. FLOUDAS, *Mathematical modeling and global optimization of large-scale extended pooling problems with the (EPA) complex emissions constraints*, Computers & Chemical Engineering, 34 (2010), pp. 1432 – 1456.
- [30] I. QUESADA AND I. GROSSMANN, *Global optimization of bilinear process networks with multi-component flows*, Computers & Chemical Engineering, 19 (1995), pp. 1219 – 1242. An International Journal of Computer Application in Chemical Engineering.
- [31] B. RIGBY, L. LASDON, AND A. WAREN, *The Evolution of Texacos Blending Systems: From OMEGA to StarBlend*, Interfaces, 25 (1995), pp. 64–83.
- [32] M. RUIZ, O. BRIANT, J.-M. CLOCHARD, AND B. PENZ, *Large-scale standard pooling problems with constrained pools and fixed demands*, Journal of Global Optimization, 56 (2012), pp. 939–956.
- [33] SYMPY DEVELOPMENT TEAM, *SymPy: Python library for symbolic mathematics*, 2016. <http://www.sympy.org> (accessed October 20, 2016).
- [34] M. TAWARMALANI AND N. V. SAHINIDIS, *Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming: Theory, Algorithms, Software, and Applications*, Kluwer Academic Publishers, Boston MA, 2002.
- [35] V. VISWESWARAN, *MINLP: applications in blending and pooling problems*, in Encyclopedia of Optimization, C. A. Floudas and P. M. Pardalos, eds., Springer US, Boston, MA, 2001, pp. 1399–1405.