SOLVING BINARY-CONSTRAINED MIXED COMPLEMENTARITY PROBLEMS USING CONTINUOUS REFORMULATIONS

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ABSTRACT. Mixed complementarity problems are of great importance in practice since they appear in various fields of applications like energy markets, optimal stopping, or traffic equilibrium problems. However, they are also very challenging due to their inherent, nonconvex structure. In addition, recent applications require the incorporation of integrality constraints. Since complementarity problems often model some kind of equilibrium, these recent applications ask for equilibrium points that additionally satisfy certain integer conditions. Obviously, this makes the problem even harder to solve. The solution approach used most frequently in the literature is to recast the complementarity conditions as disjunctive constraints using additional binary variables and big-M constraints. However, both latter aspects create issues regarding the tractability and correctness of the reformulation. In this paper, we follow the opposite route and restate the integrality conditions as complementarity constraints, leading to purely continuous reformulations that can be tackled by local solvers. We study these reformulations theoretically and provide a numerical study that shows that continuous reformulations are useful in practice both in terms of solution times and solution quality.

1. INTRODUCTION

Many real-world engineering-economic systems such as energy markets, transportation networks, or supply chains—to name just three examples—involve models with multiple, competing agents. If the principle of symmetry holds, i.e., the Jacobian of the mixed complementarity problem (MCP) function is symmetric, these systems can be modeled as a single optimization problem [18]. In this case, the assumption is that what is best for the system is also best for each participant and vice versa. For instance, in micro-economics, this is the case under the assumption of perfectly competitive markets. However, in many cases this is not realistic and, thus, a separate optimization problem for each agent is required and additional equilibrating conditions are needed to couple the optimal, self-interested decisions of every player. This situation usually leads to variational inequalities or MCPs; see, e.g., [18].

The main assumption for obtaining an MCP derived from the concatenation of separate optimization problems (and possibly additional equilibrating conditions) is that for each of the separate optimization problems, the Karush–Kuhn–Tucker (KKT) conditions [1] are both necessary and sufficient for global optimality. This usually means that the considered optimization problems are convex and that a suitable constraint qualification is satisfied. However, many important engineering-economic systems involve nonconvex models due to the modeling of the inherently nonconvex functions as part of the underlying physics (e.g., power flows in electricity [50] or

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the Weymouth equation in natural gas networks [15]) or involve integer variables (e.g., the unit commitment problem in power system dispatch models [37]).

The resulting nonconvexity of the separate optimization problems of the players makes solving them simultaneously much harder. This difficulty is due to the fact that, most often in these cases, the KKT conditions may not be necessary or sufficient for global optimality. Thus, their concatenation does not define a valid equilibrium anymore. One heuristic approach that often is applied in situations in which the nonconvexity is caused by integrality conditions in an underlying optimization problem is the following. First, all integer variables are relaxed, i.e., the continuous relaxation of the mixed-integer problem is considered. The optimal solutions of these relaxations can then be characterized by their KKT conditions assuming a constraint qualification holds. Finally, the integrality constraints are re-added to the overall resulting MCP derived from the concatenation of all KKT conditions (as well as possibly other equilibrating conditions). See [19, 21] for examples in energy and game theory as well as [42], where this approach is applied to nonconvex pricing in power markets. This approach leads to integer-valued MCPs but is heuristic since the resulting integer MCP solutions do not need to be equilibria. To provably obtain equilibria in such cases, completely different approaches need to be developed. For instance, see, e.g., [55] where algorithms are presented for computing integer-constrained Cournot equilibria. In [31], binary (quasi-)equilibria are computed by disjunctive constraints over all sets of KKT conditions. Similarly, in [57] a relaxation scheme is applied to a stylized power market and then a two-stage approach is advocated to incentivize players towards an integer-valued equilibrium.

On the other hand, there are also situations, in which the player's optimization problems can be equivalently replaced by their KKT conditions. For instance, this is the case if other nonconvex (e.g., binary) restrictions are imposed on equilibrium solutions—i.e., "after" the KKT conditions have been concatenated. Examples are certain if-then logic constraints imposed on equilibrium solutions as in the case of certain thresholds being reached or, e.g., equity-enforcement in network flows as well as integer production levels in oligopoly production models [17].

The latter cases can be modeled using MCPs with additional integrality conditions. However, these problems are much less studied compared to their continuous counterparts; see, e.g., [3, 5, 10, 38] for the linear complementarity problem (LCP) with integrality conditions. These works are of a more theoretical nature and mainly study conditions for the existence of integral LCP solutions. Moreover, there are only a few papers on algorithmic approaches for solving integer MCPs and most of the existing approaches restate the complementarity conditions using disjunctive constraints with binary variables and then solve the integer LCP by solving the resulting mixed-integer optimization problem (MIP).

In this paper, we follow the opposite approach and reformulate the integrality conditions with the help of complementarity constraints. Usually, this leads to MPEC (mathematical programs with equilibrium conditions) constraints that we then need to regularize in order to satisfy standard constraint qualifications of nonlinear optimization. This work is motivated by the median-based reformulation of discretely-constrained MCPs developed in [17]. However, instead of reformulating the resulting complementarity conditions using binary variables and then solving a MIP, as said above, we now reformulate the integrality conditions using additional complementarity constraints. The resulting purely continuous problems have the advantage that they can be tackled using local NLP solvers, which are usually faster than MIP solvers. However, this comes at the price that one typically only gets locally optimal solutions but it is reported repeatedly in the literature that similar continuous reformulations lead to very good results for practical problems [27, 33, 34, 41, 46–48, 51].

One feature of the continuous reformulations discussed in this paper is that, at least after solving the reformulation, one can decide whether the local solution is a global one. This is based on our theoretical results about that, if the continuous reformulation is solved to global optimality, we get a point that minimizes the distance to the set of continuous equilibria and to the set of integer points. Thus, if the distance is zero, this readily certifies global optimality. Depending on the specific MPEC regularization used, we obtain these minimum distances w.r.t. different norms. Finally, the continuous reformulations that we propose have the additional advantage that no big-Ms are used, whereas these constants usually need to be set heuristically in MIP reformulations of integer MCPs; see, e.g., [32, 40] for related studies on these big-M issues in bilevel optimization.

It is important to note that these discretely-constrained MCPs cannot be solved by traditional MCP solvers such as PATH [6] since PATH can "only" solve purely continuous MCPs. The focus of our paper however is on binary-constrained MCPs. Thus, this is the motivation for adjusting the formulations (median function, etc.) to be able to achieve a solution of the BC-MCP, which is a much harder problem to solve than just the continuous MCP.

The novelty of the content of this paper is twofold. First, the binary-constrained or, more generally, discretely-constrained mixed complementarity problem (DC-MCP) is a hard problem to solve and has been relatively unstudied. Some recent examples (of the co-authors) include [13, 14, 17, 19, 21, 57]. These papers discuss some useful engineering-economic applications for which the BC-MCP/DC-MCP is appropriate as related for example to (i) equity of flows in network equilibria as well as (ii) any logic constraints to such equilibrium problems. These papers showed that BC-MCP/DC-MCP is a valid class of problems to study given both the theoretical and applications-oriented focus from these papers. However, using binary variables to delineate the cases that arise from BC-MCP/DC-MCP relative to complementarity/bindingness of the constraints can be computationally challenging especially for larger problems. Thus, the current work provides a modeling alternative to the approaches specified above along with related theoretical and supporting numerical results that are very encouraging. Second, as far as we know, there has never been a numerical investigation of competing methods to solve these challenging problems considering the various solvers and formulations; see Section 4.

The remainder of this paper is organized as follows. In Section 2, we formally introduce the class of problems under consideration. For the ease of presentation, we restrict ourselves to the case of binary-constrained MCPs (BC-MCPs). Afterward, we discuss an MPEC-like continuous reformulation and three regularizations thereof as well as a median-based continuous reformulation of the BC-MCP. Afterward, we present the test set for our numerical study in Section 3 and present the numerical results in Section 4. We close the paper in Section 5 with some concluding remarks and open questions for future work.

2. Problem Formulation and Continuous Reformulations

In this section, we introduce the bounded mixed complementarity problem; cf., e.g., [11]. To this end, let the function $F : \mathbb{R}^n \to \mathbb{R}^n$ and the vectors $l, u \in$

$\mathbb{R}^n \cup \{-\infty, +\infty\}$ with $l \leq u$ be given, where the latter inequality is meant componentwise. The problem is then to find a vector $z \in \mathbb{R}^n$ that satisfies

$$F_i(z) \geq 0 \quad \text{if } z_i = l_i, \tag{1a}$$
$$F_i(z) = 0 \quad \text{if } l_i < z_i < u_i, \tag{1b}$$
$$F_i(z) \leq 0 \quad \text{if } z_i = u_i. \tag{1c}$$

For what follows, we also introduce the more traditional form of stating an MCP, in which the vector z is split up into a nonnegative vector $0 \leq x \in \mathbb{R}^{n_x}$ with respective nonnegative entries F_i of F as well as the remaining variables $y \in \mathbb{R}^{n_y}$, which are free, and the associated entries F_i are considered to be equations. More formally, the traditional MCP is to find vectors (x, y) that satisfy

$$0 \leq F_i(x, y) \perp x_i \geq 0, \quad i \in I_x = \{1, \dots, n_x\}, \tag{2a}$$
$$0 = F_j(x, y), \ y_j \text{ free}, \quad j \in I_y = \{1, \dots, n_y\}. \tag{2b}$$

Here and in what follows, we use the notation $a \perp b$ meaning that the vectors a and b are orthogonal to each other. Note that (2) is the special case of (1) with

$$l_i = 0, \ u_i = \infty, \quad i \in I_x,$$
$$l_j = -\infty, \ u_j = \infty, \quad j \in I_y,$$

and $z^\top = (x^\top, y^\top)$ as well as $I_x \cup I_y = \{1, \dots, n\}$.

The binary-constrained mixed complementarity problem (BC-MCP) is to find a vector $z \in \mathbb{R}^n$ that satisfies (1) and the additional constraints

$$z_i \in \{0, 1\}, \quad i \in D \subseteq \{1, \dots, n\}. \tag{3}$$

Similar formulations can also be found in [13, 14, 19, 21]. Translated to the formulation (2) this corresponds to additionally requiring $z_i \in \{0, 1\}$ for $i \in D_x \subseteq I_x$ since all binary variables automatically correspond to the index set I_x.

Formally, a BC-MCP solution is a vector z that satisfies (1) and (3). Both for classical continuous complementarity problems and its pure integer variant, the question of existence of solutions is well studied; see, e.g., the seminal textbook [4] or [3, 5, 10, 38, 52] for the discussion of integer LCPs. Unfortunately, it turns out that the conditions for existence of integer LCP solutions are rather strong. The last group of papers consider purely integer LCPs. Integer nonlinear complementarity problems are studied, in, e.g. [35, 58].

2.1. **MPEC-Based Continuous Reformulations of the BC-MCP.** In what follows, we derive continuous reformulations of the BC-MCP. To this end, we first observe that we can reformulate the alternatives in (1) using the system of inequalities

$$(z_i - l_i)F_i(z) \leq 0, \quad i \in \{1, \dots, n\}, \tag{4a}$$
$$(u_i - z_i)F_i(z) \geq 0, \quad i \in \{1, \dots, n\}, \tag{4b}$$
$$z_i \in [l_i, u_i], \quad i \in \{1, \dots, n\}, \tag{4c}$$

for which we additionally need to assume $l_i < u_i$ for each $i \in \{1, \dots, n\}$. Thus, a BC-MCP solution is a point satisfying (3) and (4). To see why the assumption $l_i < u_i$ for each i is required, we consider the following three cases:

(i) $l_i < z_i < u_i$,
(ii) $z_i = l_i \leq u_i$, and
(iii) $z_i = u_i \geq l_i$.

In Case (i), (4a) implies that $F_i(z) \leq 0$ and (4b) leads to $F_i(z) \geq 0$, which together give (1b). In Case (ii), (4a) does not restrict $F_i(z)$ at all and (4b) only implies $F_i(z) \geq 0$ if $l_i < u_i$. Thus, we need the assumption $l_i < u_i$ to ensure that (1a) holds.

Lastly, in Case (iii), both (4a) and (4b) do not impose any restrictions on $F_i(z)$ unless $l_i < u_i$. However, if $l_i < u_i$ holds, we obtain (1c). Thus, unless otherwise noted, for the BC-MCP we assume in the following that $l_i < u_i$ for all i.

We now start deriving purely continuous reformulations of the BC-MCP. The key to the first family of such reformulations is the obvious observation that $z_i \in \{0, 1\}$ is equivalent to

$$z_i \in [0, 1] \subseteq \mathbb{R}, \quad z_i(1 - z_i) = 0.$$

Thus, we can replace the BC-MCP equivalently by

$$(z_i - l_i)F_i(z) \leq 0, \quad i \in \{1, \dots, n\}, \tag{5a}$$
$$(u_i - z_i)F_i(z) \geq 0, \quad i \in \{1, \dots, n\}, \tag{5b}$$
$$z_i \in [l_i, u_i], \quad i \in \{1, \dots, n\}, \tag{5c}$$
$$0 \leq (1 - z_i) \perp z_i \geq 0, \quad i \in D. \tag{5d}$$

The MPEC-like condition (5d) is again a complementarity problem, which means that we still remain in the original class of problems compared to the original, i.e., continuous, MCP (1). We will refer to this formulation as the complementarity-constrained formulation (CCF).

We note that in order to solve CCF it is possible to directly apply nonlinear optimization (NLP) solvers to System (5), interpreted as the constraint set of an optimization problem with an arbitrary objective function. However, the complementarity structure always leads to a violation of classical constraint qualifications (CQ) for NLPs like the linear independence CQ (LICQ) or the Mangasarian–Fromowitz CQ (MFCQ); see, e.g., [59]. In what follows, we apply standard regularization techniques that tackle this lack of constraint regularity. However, since we now have the MPEC reformulation (5) at hand, which will be the basis of what follows, we first comment on treating general, integer-valued variables. While System (5) is stated for binary-constrained MCPs, it can easily be extended to more general integer-constrained MCPs using binary expansions.

As just mentioned before, from an optimization point of view, constraints like in (5d) are typically complicating the problem since classical CQs like LICQ or MFCQ are violated at all feasible points. As a consequence, a rather large branch of research evolved in the last decades that studies MPEC-specific regularizations of these constraints. In what follows we discuss two of them:

(i) the regularization of Scholtes [29, 49], and
(ii) the penalization approach [30].

We start with the regularization of Scholtes, which relaxes the MPEC constraint so that (5) is replaced with

$$(z_i - l_i)F_i(z) \leq 0, \quad i \in \{1, \dots, n\}, \tag{6a}$$
$$(u_i - z_i)F_i(z) \geq 0, \quad i \in \{1, \dots, n\}, \tag{6b}$$
$$z_i \in [l_i, u_i], \quad i \in \{1, \dots, n\}, \tag{6c}$$
$$z_i(1 - z_i) \leq \varepsilon, \quad i \in D, \tag{6d}$$
$$z_i \in [0, 1], \quad i \in D, \tag{6e}$$

where $\varepsilon > 0$ is a given regularization parameter. We will refer to this relaxed complementarity-constrained problem as RCCF-ε. Obviously, we recover the original BC-MCP for $\varepsilon = 0$ and the constraint subset (6d)–(6e) concerned with the complementarity reformulation of the binary variables indeed satisfies the LICQ for small enough ε under suitable assumptions; see, e.g., Lemma 2.1 in [49]. Note that in (6) any objective function can be used on top of the stated conditions to solve the corresponding optimization function.

We can solve Problem (6) by fixing the parameter ε and by using general-purpose solvers for nonlinear optimization. Let us note that 0.25 is an upper bound of the left-hand side in (6d) under the additional constraint (6e). After solving the problem, if the binary enforcing complementarity constraint (5d), i.e.,

$$0 \leq (1 - z_i) \perp z_i \geq 0,$$

holds for all i, then the solution is a BC-MCP solution. If this constraint is not satisfied, these problems often are solved with homotopy-like methods that solve a series of ε_k-regularized problems of type (6) while driving down the regularization parameters to zero. For further details, we refer the interested reader to [29] and [45].

As mentioned before, the conditions ensuring the existence of integer LCP solutions are rather strong. Although the existence of solutions of BC-MCPs as considered in this paper is still an open research question, the results on integer LCPs indicate that analogous conditions will not be weaker in the case of BC-MCPs. Fortunately, in the case of non-existence of solutions, we can use the Scholtes-like regularization (6) for computing the minimum ℓ_∞-norm distance of a continuous MCP solution to a binary solution by solving the optimization problem

$$\min_{z,\varepsilon} \quad \varepsilon \tag{7a}$$

$$\text{s.t.} \quad (z_i - l_i)F_i(z) \leq 0, \quad i \in \{1, \dots, n\}, \tag{7b}$$

$$(u_i - z_i)F_i(z) \geq 0, \quad i \in \{1, \dots, n\}, \tag{7c}$$

$$z_i \in [l_i, u_i], \quad i \in \{1, \dots, n\}, \tag{7d}$$

$$z_i(1 - z_i) \leq \varepsilon, \quad i \in D, \tag{7e}$$

$$z_i \in [0, 1], \quad i \in D. \tag{7f}$$

We call this problem RCCF-ε-opt in the following. It is a nonconvex problem and thus, in general, hard to solve.

Note that in (7), the optimal ε will take the value of the maximum $z_i(1 - z_i)$ over all $i \in D$, since ε is being minimized and $\varepsilon \geq z_i(1 - z_i)$ for all $i \in D$ due to constraint (7e). In addition, the closer the value of z_i in the maximum of $z_i(1 - z_i)$ over all i is to 0 or 1, the smaller ε will be. Obviously, the maximum of $z_i(1 - z_i)$ over all i can take value 0 only in case that all z_i are equal to 0 or 1. Thus, by construction, we obtain the following result.

Theorem 1. *Let $\mathcal{S}$ be the solution set of (1), i.e., $\mathcal{S} = \{z \in \mathbb{R}^n : z$ satisfies (1)$\}$. Moreover, let $\mathcal{B} = \{z \in \mathbb{R}^n : z_i \in \{0, 1\}$ for all $i \in D\}$. If (z^*, ε^*) is an optimal solution of Problem (7), then*

$$z^* \in \arg\min\{\|z - z'\|_\infty : z \in \mathcal{S},\ z' \in \mathcal{B}\}.$$

In particular, z^* is a BC-MCP solution if and only if (z^*, ε^*) with $\varepsilon^* = 0$ is a solution of Problem (7).

Let us note that "solution" in the latter theorem means a global optimal solution. However, (7) is a nonconvex problem so a global solution might be hard to obtain in practice.

We next discuss regularization by penalization. Here, the MPEC constraints are directly removed from the set of constraints and get penalized in the objective function. Thus, the problem to solve, which we will refer to as RCCF-pen, reads

$$\min_{z} \quad \sum_{i \in D} z_i(1 - z_i) \tag{8a}$$
$$\text{s.t.} \quad (z_i - l_i)F_i(z) \le 0, \quad i \in \{1, \dots, n\}, \tag{8b}$$
$$(u_i - z_i)F_i(z) \ge 0, \quad i \in \{1, \dots, n\}, \tag{8c}$$
$$z_i \in [l_i, u_i], \quad i \in \{1, \dots, n\}, \tag{8d}$$
$$z_i \in [0, 1], \quad i \in D. \tag{8e}$$

Note that we moved the nonconvexity of the constraints (6d) to the objective function in Problem (8). One question later in our numerical study will thus also be to find out whether it is easier in practice to handle this nonconvexity in the constraints or in the objective function. However, removing the constraints that violate standard CQs from the constraint set directly leads to an increase of constraint regularity in terms of CQs.

Again, it can be easily observed that, the closer each z_i is to 0 or 1, the smaller each term of the objective function and therefore, the smaller the objective function. This is because each $z_i \in [0, 1]$ rather than in $[0, \infty)$. Furthermore, each term of the objective function can take value 0 just in the case in which the corresponding z_i takes exactly value 0 or 1. Hence, again by construction, we obtain the following result.

Theorem 2. *Let $\mathcal{S}$ be the solution set of (1), i.e., $\mathcal{S} = \{z \in \mathbb{R}^n : z$ satisfies (1)$\}$. Moreover, let $\mathcal{B} = \{z \in \mathbb{R}^n : z_i \in \{0, 1\}$ for all $i \in D\}$. If z^* is an optimal solution of Problem (8), then*

$$z^* \in \arg\min\{\|z - z'\|_1 : z \in \mathcal{S},\ z' \in \mathcal{B}\}.$$

In particular, z^* is a BC-MCP solution if and only if $\sum_{i \in D} z_i^*(1 - z_i^*) = 0$ holds.

Formulations (7) and (8) can be solved by applying general-purpose NLP solvers. Although those usually only provide locally optimal solution, we know by Theorem 1 and 2 that if and only if the solver reports an optimal value of 0, we have found a solution of the original BC-MCP.

It is, of course, also possible to apply other MPEC-regularization techniques to the reformulation (5). Prominent further examples are approaches using the Fischer–Burmeister function or the min-function; cf., e.g., [12, 53]. However, due to our preliminary numerical experiments and our experience in related fields [45], we restrict ourselves to the above two regularizations.

We close this section with some remarks on the special case of binary-constrained mixed linear complementarity problems. In this case, (7) is a quadratically constrained optimization problem (QCP) and (8) is a quadratically constrained quadratic program (QCQP). For both problems, the constraints (7b) and (7c) as well as (8b) and (8c) are convex if and only if the square matrix M of the affine-linear function $F(z) = Mz + q$ is positive semidefinite. However, the constraints (7e) as well as the objective function (8a) are always nonconvex as discussed above. Thus, although we get rid of the binary variables, the problems to be solved are still hard, nonconvex optimization problems.

2.2. **Median-Based Reformulation of the BC-MCP.** As described in [16] and [20], the bounded MCP can be equivalently recast as finding the zero of the function $H : \mathbb{R}^n \to \mathbb{R}^n$ defined by

$$H_i(z) := z_i - \operatorname{mid}\{l_i, u_i, z_i - F_i(z)\} \quad \text{for all } i \in \{1, \dots, n\}, \tag{9}$$

where $\operatorname{mid}\{a, b, c\}$ represents the median of the three scalars a, b, c.

We now consider the median function H given in (9) and the related optimization problem

$$\min_{z} \quad \|H(z)\| \tag{10a}$$
$$\text{s.t.} \quad z_i \in [l_i, u_i], \quad i \in \{1, \dots, n\}, \tag{10b}$$
$$z_i \in \{0, 1\}, \quad i \in D, \tag{10c}$$

where $\|\cdot\|$ is any vector norm. It is shown in [17] that a point z is a BC-MCP solution if it solves (10) with optimal objective function value 0. Moreover, in the latter paper it is also shown that using the ℓ_1-norm and a set of disjunctive constraints using binary variables based on the cases of the median function in (9), an equivalent mixed-integer linear program can be formulated.

One problem with this median MIP formulation is that it contains many binary variables and big-M constraints, which makes it hard to solve. Thus, we propose an alternative formulation to solve problem (10) by using continuous variables and complementarity constraints. The main idea is to use these new variables and constraints to address the different possible cases of the median function. Since two of the arguments of the median function are ordered ($l \leq u$) we only need to consider the following three cases for each component $i \in \{1, \dots, n\}$:

(a) $z_i - F_i(z) \leq l_i \leq u_i$, which implies $H_i(z) = z_i - l_i$,
(b) $l_i \leq u_i \leq z_i - F_i(z)$, which implies $H_i(z) = z_i - u_i$,
(c) $l_i \leq z_i - F_i(z) \leq u_i$, which implies $H_i(z) = F_i(z)$.

In the following formulation, the variables b_i^1, b_i^2, and b_i^3 refer to the three different possible cases of the median function described above, respectively.

$$\min_{z,b,\mu} \quad \|(\mu_1, \dots, \mu_n)^\top\| \tag{11a}$$
$$\text{s.t.} \quad z_i \in [l_i, u_i], \quad i \in \{1, \dots, n\}, \tag{11b}$$
$$z_i(1 - z_i) = 0, \ z_i \in [0, 1], \quad i \in D, \tag{11c}$$
$$\big(l_i - (z_i - F_i(z))\big)b_i^1 \geq 0, \quad i \in \{1, \dots, n\}, \tag{11d}$$
$$\big(z_i - F_i(z) - u_i\big)b_i^2 \geq 0, \quad i \in \{1, \dots, n\}, \tag{11e}$$
$$\big(z_i - F_i(z) - l_i\big)b_i^3 \geq 0, \quad i \in \{1, \dots, n\}, \tag{11f}$$
$$\big(u_i - (z_i - F_i(z))\big)b_i^3 \geq 0, \quad i \in \{1, \dots, n\}, \tag{11g}$$
$$b_i^1 + b_i^2 + b_i^3 = 1, \quad i \in \{1, \dots, n\}, \tag{11h}$$
$$\mu_i = z_i - \big(b_i^1 l_i + b_i^2 u_i + b_i^3 (z_i - F_i(z))\big), \quad i \in \{1, \dots, n\}, \tag{11i}$$
$$b_i^j (1 - b_i^j) = 0, \quad i \in \{1, \dots, n\}, \ j = 1, 2, 3, \tag{11j}$$
$$b_i^j \in [0, 1], \quad i \in \{1, \dots, n\}, \ j = 1, 2, 3. \tag{11k}$$

We will refer to formulation (11) as the CCF-median formulation. Note that this formulation does not require the use of big-Ms, unlike the formulation with median-related binary variables proposed in [17]. However, this comes at the price of additional nonconvex constraints. As we did in the last section, we could also regularize the complementarity constraints in (11c) and (11j). However, since the median-based formulation already has an objective function we would need to put a weight on the penalization terms.

By construction of the problem, we get the following theorem.

Theorem 3. *An optimal solution (z, b, μ) of (11) has an objective function value of 0 if and only if z is a BC-MCP solution.*

Proof. We start by showing that if (z, b, μ) is an optimal solution of (11) with objective function value 0, then z is a BC-MCP solution. To this end, let (z, b, μ)

be an optimal solution of (11) with objective function value 0. In the following, we prove that this implies that z solves (10) with an objective value of 0, which itself implies, as referred before, that z solves the original BC-MCP problem.

First, if z satisfies (11b) and (11c), it obviously satisfies (10b) and (10c). Second, we show that $\mu_i = H_i(z)$ for all $i \in \{1, \dots, n\}$ and, thus, $\|H(z)\| = \|\mu\| = 0$. For doing so, we consider the different possible values that the vector b can take. By Constraints (11j) and (11k), each $b_i^j \in \{0, 1\}$ for $i \in \{1, \dots, n\}$ and $j = 1, 2, 3$. Moreover, by Constraint (11h), for each $i \in \{1, \dots, n\}$, $b_i^j = 1$ for exactly one $j \in \{1, 2, 3\}$. We distinguish for each $i \in \{1, \dots, n\}$ the three different possible cases depending on the values of b_i^1, b_i^2, and b_i^3:

(i) $b_i^1 = 1$, $b_i^2 = b_i^3 = 0$. This implies, by Constraint (11d), that $(l_i - (z_i - F_i(z))) \geq 0$, and hence, since by assumption $l_i \leq u_i$, we are in the case $H_i(z) = z_i - l_i$. Furthermore, Constraint (11i) implies $\mu_i = z_i - l_i = H_i(z)$.

(ii) $b_i^1 = 0$, $b_i^2 = 1$, $b_i^3 = 0$. Constraint (11e) implies $(z_i - F_i(z) - u_i) \geq 0$ and this implies $l_i \leq u_i \leq z_i - F_i(z)$. Thus, we are in the case $H_i(z) = z_i - u_i$. Additionally, by Constraint (11i), we obtain $\mu_i = z_i - u_i = H_i(z)$.

(iii) $b_i^1 = 0 = b_i^2$, $b_i^3 = 1$. Constraints (11f) and (11g) implies $(z_i - F_i(z) - l_i) \geq 0$ and $(u_i - (z_i - F_i(z))) \geq 0$, which means we have $H_i(z) = F_i(z)$. Finally, by Constraint (11i), we obtain $\mu_i = F_i(z)$, which shows $H_i(z) = \mu_i$.

We are still left with proving the inverse implication: If z is a BC-MCP solution then, there exist b and μ such that (z, b, μ) is an optimal solution of (11) with objective function value 0. To this end, let z be a BC-MCP solution. Thus, z is an optimal solution of (10) with objective value 0. The construction of b and μ depends on the value of the median function. For each $i \in \{1, \dots, n\}$, if we are in Case (a) (cf. before Problem (11)) for i, then we take $b_i^1 = 1$, $b_i^2 = 0$, and $b_i^3 = 0$. Hence, $\mu_i = z_i - l_i$. Instead, if we are in Case (b) for i, we set $b_i^1 = 0$, $b_i^2 = 1$, and $b_i^3 = 0$ and, hence, $\mu_i = z_i - u_i$. Otherwise, if we are in Case (c) for i, we set $b_i^1 = 0$, $b_i^2 = 0$, and $b_i^3 = 1$. Thus, $\mu_i = F_i(z)$. If different cases hold simultaneously, we simply construct the solution of one of the respective cases.

It can be easily checked that the constructed solution (z, b, μ) verifies all the constraints in (11) and $\mu = H(z)$. Thus, $\|\mu\| = 0$. □

3. Test Problems

In this section, we describe the test problems used for the computational experiments presented in the next section to compare the different proposed reformulations. Unfortunately, there are no general-purpose test sets for (discretely-constrained) MCPs in the literature. Thus, we need to construct our own instances and, for doing so, we mainly follow the construction of test problems in [17]. Our entire test set is split up into three groups:

(1) Randomly generated instances for which we know that a binary solution exists by construction; see Section 3.1.
(2) Randomly generated instances for which we do not know that a binary solution exists; see Section 3.1 as well.
(3) Instances for spatial price equilibrium problems on different bipartite networks with linear and quadratic transportation cost functions as well as additional if-then logic constraints; see Section 3.2.

Table 1 gives an overview over the test problems. We set the maximum sizes of the different instances as large as possible. This means that our preliminary numerical experiments revealed that only very few instances of bigger size can be solved.

3.1. **Random Instances.**

We construct random BC-MCP instances as follows so that the existence of a binary solution is guaranteed. First, a vector $\bar{z}^\top = (\bar{x}^\top, \bar{y}^\top)$

TABLE 1. Summary of Test Instances

ID	binary variables	continuous variables	Binary solution guaranteed?	Type of Problem
1	500	500	yes, by construction	large random
	700	700	yes, by construction	large random
2	500	500	no	large random
	700	700	no	large random
3, 4	20	800	no	spatial price equilibrium
	25	1250	no	spatial price equilibrium

is generated randomly, with $\bar{x}$ being a vector with components in $\{0, 1\}$ and $\bar{y}$ is a continuous vector taking values in $[-50, 50]$. Then, a square matrix

$$M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}$$

is generated mainly following the construction used in [17] but with restricted density of the matrix, i.e., we set $M_{ij} = (i+j)/2$ for a fraction of $\rho \in [0, 1]$ randomly chosen entries. All other entries are set to zero. Afterward, the vector q is computed as $q = -M\bar{z}$ so that the vector $\bar{z}$ is a binary-feasible solution of the MCP (2) with $F(z) = q + Mz$.

For our computational study we will use instances of the following sizes:

- $I_x = D_x = \{1, \dots, 500\}$ and $I_y = \{1, \dots, 500\}$,
- $I_x = D_x = \{1, \dots, 700\}$ and $I_y = \{1, \dots, 700\}$.

The second type of instances is constructed in exactly the same way but we choose $\bar{x} \in [0, 1]$ instead of $\bar{x} \in \{0, 1\}$. Thus, for the second set of test problems it is not guaranteed that a binary solution exists.

3.2. **Spatial Price Equilibrium Problems with If-Then Logic Constraints.** The spatial price equilibrium problem (SPE) is a generalization of the classical transportation problem [18, 28, 44]. For the ease of implementation and presentation, we consider the SPE on complete bipartite networks of spatially dispersed supply nodes $i \in I$ and demand nodes $j \in J$ as well as a set of connecting arcs $a \in A = \{(i, j) \colon i \in I, j \in J\}$. The goal is to determine a vector of nonnegative flows $0 \leq x = (x_{ij})_{(i,j) \in A}$ such that

$$0 \leq \Psi_i \left(\sum_{j \in J} x_{ij} \right) + c_{ij}(x_{ij}) - \theta_j \left(\sum_{i \in I} x_{ij} \right) \perp x_{ij} \geq 0 \quad \text{for all } i \in I,\ j \in J, \quad (12)$$

where

$$\Psi_i \left(\sum_{j \in J} x_{ij} \right), \quad c_{ij}(x_{ij}), \quad \theta_j \left(\sum_{i \in I} x_{ij} \right)$$

are the inverse supply function (defining the supply price as a function of the total supply $\sum_{j \in J} x_{ij}$ at node i), the transportation cost function, and the inverse demand function (defining the demand price as a function of the total demand $\sum_{i \in I} x_{ij}$ at node j), respectively. Here,

$$F_{ij}(x) = \Psi_i \left(\sum_{j \in J} x_{ij} \right) + c_{ij}(x) - \theta_j \left(\sum_{i \in I} x_{ij} \right) \quad \text{for all } (i, j) \in A$$

are the components of the MCP function $F : \mathbb{R}^{|A|} \to \mathbb{R}^{|A|}$. Thus, the SPE is an instance of an MCP with only nonnegative variables.

Additionally, we assume the following logic that is used to enforce some kind of equity in the network:

$$\text{if} \quad \sum_{j\in J} x_{ij} < \delta_i \quad \text{then} \quad \sum_{j\in J} x_{ij} \geq \gamma \sum_{i\in I}\sum_{j\in J} x_{ij} \quad \text{for all } i \in I,$$

where δ_i is some minimum contractual threshold for supply guaranteed to the supplier at node $i \in I$. This if-then condition can be read as follows: If the equilibrium flow out of supply node i is less than the contractual minimum, then the ith energy supply node gets at least a fraction of $\gamma \in [0, 1]$ of the total flow. Such conditions can be implemented by adding the constraints

$$\delta_i - \sum_{j\in J} x_{ij} \leq b_i M_i, \tag{13a}$$

$$-\sum_{j\in J} x_{ij} + \gamma \sum_{i\in I}\sum_{j\in J} x_{ij} \leq M_i'(1 - b_i), \tag{13b}$$

$$b_i \in \{0, 1\}. \tag{13c}$$

for all $i \in I$. Here, M_i, M_i', $i \in I$, are positive constants chosen sufficiently large to ensure the correctness of the formulation. Using the assumptions on the functions of the SPE that we discuss next, we can derive provably correct big-M values; see Appendix A. We consider this kind of if-then logic constraint here as a prototype. Other logical constraints can be incorporated in similar ways. In order to deal with constraint (13c), we derive purely continuous reformulations using the same techniques as in (5), (6)–(8), or (11).

Finally, we need to specify how we choose the transportation cost, the inverse supply, and the inverse demand functions. For the ease of implementation, we again restrict ourselves to the linear case. Thus, the inverse supply functions are of the form

$$\Psi_i\left(\sum_{j\in J} x_{ij}\right) = \rho_i \sum_{j\in J} x_{ij} + \gamma_i \quad \text{for all } i \in I,$$

the inverse demand functions are given by

$$\theta_j\left(\sum_{i\in I} x_{ij}\right) = -\rho_j' \sum_{i\in I} x_{ij} + \gamma_j' \quad \text{for all } j \in J,$$

and the transportation cost functions are assumed to be linear,

$$c_{ij}(x_{ij}) = \omega_{ij} x_{ij} \quad \text{for all } i \in I,\ j \in J,$$

or quadratic,

$$c_{ij}(x_{ij}) = \omega_{ij} x_{ij}^2 \quad \text{for all } i \in I,\ j \in J.$$

Note that in the case in which the transportation costs are quadratic, the function F is quadratic as well. The constants ρ_i, γ_i, ω_{ij}, ρ_j', γ_j' are all chosen positive such that the supply and demand functions as well as the transportation cost functions satisfy the conditions of Proposition 7.10 in [28]. Thus, existence of solutions is guaranteed. This means, $\Psi_i(\sum_j x_{ij}) \geq 0$ as well as $c_{ij}(x_{ij}) \geq 0$ are monotonically increasing and $\theta_i(\sum_j x_{ij})$ is monotonically decreasing. However, note that existence of solutions is only guaranteed in the purely continuous case. If the if-then logic constraints (13) are imposed in addition, there might be no binary-constrained equilibrium point.

In the numerical results presented in the next section, we consider instances of if-then logic constrained SPEs on complete bipartite graphs with $|I| = 20$, $|J| = 40$ as well as $|I| = 25$, $|J| = 50$. Thus, we will have 20 or 25 binary variables, respectively.

4. Numerical Results

We now discuss the numerical results for the different test problems presented in Section 3. The computational study has been done using a computer with two Intel(R) Xeon(R) E5-2699 v4 CPUs with 2.2 GHz, 44 physical cores, and 756 GB RAM. All models are implemented using GAMS version 28.2.0 [22]. The only MINLP formulation, namely the BC-MCP, is solved using the global MINLP solvers SCIP version 6.0 [25], BARON version 19.7.13 [43, 54], ANTIGONE version 1.1. [36], and the local MINLP solver KNITRO version 11.1.1 [2]. For the continuous reformulations CCF, RCCF-ε, RCCF-ε-opt, and RCCF-pen we also used KNITRO version 11.1.1, as well as the local NLP solvers CONOPT4 version 4.12 [7–9], SNOPT version 7.2-12.1 [23, 24], and Ipopt version 3.12 [56]. We always used the default initial values of GAMS, the default options of all solvers, and a time limit of 300 seconds since our preliminary numerical experiments revealed that a larger time limit does not lead to significantly more solved instances. The parameter ε in RCCF-ε is always set to 0.25.

Note that in the cases in which the only nonlinear constraints in the BC-MCP formulation are the complementarity constraints, the instances can, in principle, also be solved by using mixed-integer linear programming (MILP) solvers and their built-in functionality to handle disjunctive constraints. We tried to solve all the proposed instances of type 1 using the MILP solver GUROBI v. 9 [26]. However, none of the instances could be solved within the time limit. Even for a time limit increased by the factor 20, no instance could be solved with this approach. For this reason, we exclude a further comparison of these MILP-based approaches in the following.

The following sections will present detailed discussions of the numerical results for the different continuous reformulations applied to the different test sets. The main results will be the following:

(1) The median-based continuous reformulation is not competitive to the other continuous reformulations.
(2) The special structure of the instances for which a binary solution is guaranteed seems to be detected and exploited well by the global solvers whereas this is not the case for the local solvers.
(3) The performance strongly depends on the combination of the chosen continuous reformulation and the chosen local solver.
(4) KNITRO and Ipopt perform very good when applied to the RCCF-ε-opt and RCCF-pen models. Using these combinations outperforms the global solvers applied to the mixed-binary BC-MCP formulation for almost all instances.

4.1. **Discussion of the Numerical Results of the Median-Based Reformulation.** We start by discussing the numerical results of the median-based reformulation (11). We include the median-based reformulation for the sake of completeness and to compare the proposed MPEC-based reformulations with this approach that is based on an existing reformulation of the BC-MCP in the literature. However, although theoretically appealing, the median-based continuous reformulation is not competitive from a computational point of view. In our numerical experiments, we used the squared ℓ_2-norm in (11a). The results are as follows: None of the considered local NLP solvers can find a BC-MLCP solution for the random instances with guaranteed binary solution (see Section 3.1) within the time limit using the median-based reformulation. This is in clear contrast to the numerical results obtained for the other continuous reformulations and also in contrast to the results of the mixed-integer reformulation of the median-based model as reported in [17].

TABLE 2. Numerical results for random instances type 1 for the BC-MCP formulation

	$n_x = 500$, $n_y = 500$				$n_x = 700$, $n_y = 700$			
	$\rho = 0.15$		$\rho = 0.25$		$\rho = 0.15$		$\rho = 0.25$	
Solver	Opt	Time	Opt	Time	Opt	Time	Opt	Time
BARON	25	35.74	25	44.31	22	83.66	19	92.75
SCIP	25	5.62	25	6.88	25	15.81	25	19.04
ANTIGONE	25	21.98	25	28.46	25	105.92	25	115.12
KNITRO	25	52.02	22	41.67	23	144.79	25	251.86

TABLE 3. Numerical results for random instances type 1, $n_x = 500$, $n_y = 500$, and $\rho = 0.15$

	CCF		RCCF-ε			RCCF-ε-opt			RCCF-pen		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	0	—	14	14	39.18	25	25	41.43	25	25	36.83
CONOPT4	6	140.53	0	0	—	0	0	—	0	0	—
SNOPT	0	—	0	0	—	0	0	—	0	0	—
Ipopt	22	73.81	0	0	—	12	12	102.71	1	1	43.17

TABLE 4. Numerical results for random instances type 1, $n_x = 500$, $n_y = 500$, and $\rho = 0.25$

	CCF		RCCF-ε			RCCF-ε-opt			RCCF-pen		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	0	—	11	11	50.2	23	23	47.04	25	25	42.66
CONOPT4	11	150.51	0	0	—	0	0	—	0	0	—
SNOPT	25	12.05	25	25	11.92	0	0	—	0	0	—
Ipopt	23	92.03	0	0	—	9	9	96.74	1	1	108.58

A possible reason for this may be the complexity of the model. By simply counting the number of nonlinearities, complementarity constraints, or variables it can be expected that the median-based reformulation is harder to solve compared to the other continuous reformulations CCF, RCCF-ε, RCCF-ε-opt, and RCCF-pen.

Due to these results we do not include results for the median-based reformulation in the discussions of the following sections.

4.2. **Numerical Results for Random Instances.** For the randomly generated instances of type 1 (binary solutions guaranteed) and 2 (no binary solutions guaranteed) described in Section 3.1, we generated 25 random instances for each size ($|I_x| = 500$, $|I_y| = 500$ and $|I_x| = 700$, $|I_y| = 700$) and each density parameter $\rho \in \{0.15, 0.25\}$. In the numerical experiments, all applicable solvers are applied to all reformulations for all instances of type 1 and 2. The numerical results for all type 1 instances are shown in Tables 2–6 and Tables 7–10 contain the results for all instances of type 2.

4.2.1. *Type-1 Instances.* In Table 2, we show the number of instances solved to optimality ("Opt") within the time limit and the average running times ("Time"; always denoted in seconds) for solving the instances using the BC-MCP, i.e., the

Table 5. Numerical results for random instances type 1, $n_x = 700$, $n_y = 700$, and $\rho = 0.15$

	CCF		RCCF-ε			RCCF-ε-opt			RCCF-pen		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	0	—	15	15	130.51	23	23	84.31	25	25	92.79
CONOPT4	0	—	0	0	—	0	0	—	0	0	—
SNOPT	0	—	0	0	—	0	0	—	0	0	—
Ipopt	19	207.93	0	0	—	6	6	198.04	1	1	247.19

Table 6. Numerical results for random instances type 1, $n_x = 700$, $n_y = 700$, and $\rho = 0.25$

	CCF		RCCF-ε			RCCF-ε-opt			RCCF-pen		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	0	—	12	12	106.68	23	23	112.73	23	23	82.59
CONOPT4	0	—	0	0	—	0	0	—	0	0	—
SNOPT	25	36.55	25	25	28.35	3	3	192.95	0	0	—
Ipopt	20	183.73	0	0	—	8	8	177.35	1	1	184.77

mixed-integer formulation. The table shows the results for different instance sizes, two different density parameters ρ, and for all applied solvers. Here and in what follows, average times are always taken only over those instances that are solved within the time limit.

In Tables 3–6, we report the same information for the four tested continuous reformulations. Note that solving the reformulations RCCF-ε, RCCF-ε-opt, and RCCF-pen do not need to result in binary feasible solutions of the original BC-MCP. Thus, we additionally report the number of instances for which such a "solution" is also binary-feasible ("BF").

We can observe in Table 2 that almost all instances using the mixed-integer BC-MCP formulation are solved in less than 300 seconds. SCIP solves all instances, is always the fastest solver, and never requires more than 20 seconds in average. Most of the global solvers find a solution in the preprocessing phase or at the root node. The reason might be the simple structure of the instances, for which by construction, a solution can be found by solving a linear system of equations. The overall picture regarding running times is as expected: The larger and the more dense an instance is, the harder it is to solve.

In contrast to the tested MINLP solvers, the special structure of the instances is not exploited by the local solvers. This is also to be expected since global solvers usually involve a much more sophisticated preprocessing than local solvers. Let us discuss the results of the local solvers in more detail. Using KNITRO for the continuous reformulations RCCF-ε-opt and RCCF-pen, it is possible to compute a BC-MCP solution for almost all of the instances. For example, for 500 binary and continuous variables as well as $\rho = 0.15$ (Table 3), a BC-MCP solution is found in 36.83 seconds on average using the RCCF-pen model, whereas it takes 42.66 seconds for $\rho = 0.25$ (Table 4). Thus, KNITRO applied to the continuous reformulations is competitive to all global solvers except for SCIP, which always finds a BC-MCP solution at the root node.

The other results are rather surprising. CONOPT4 is only able to compute solutions for the smaller set of instances and does not benefit from the MPEC-regularizations at all: The only instances that are solved are CCF models. Moreover, the CCF and RCCF-ε formulations perform well when solved with SNOPT—however, only in the case in which the matrix M is more dense ($\rho = 0.25$). In this case, all instances are solved very fast to a BC-MCP solution. For example, we can observe in Table 6 that the average time to find a BC-MCP solution is 36.55 and 28.35 seconds for CCF and RCCF-ε, respectively. Note that these times are rather close to the solution time required for SCIP in the BC-MCP formulation. However, for reduced matrix density, SNOPT is not able to compute a single binary-feasible solution—which is a very surprising result. Regarding the remaining applicable solvers for these two formulations, we can observe in Tables 3–6 that CCF performed reasonable well with Ipopt: more than 80 % of the instances can be solved but Ipopt requires large running times in general. More than 50 % of the instances are solved to a BC-MCP solution with solver KNITRO and the RCCF-ε approximation. However, as already discussed above, KNITRO performs best when applied to the RCCF-ε-opt and RCCF-pen models.

In conclusion for these test instances, the global solvers, especially SCIP, can solve the mixed-integer BC-MCP formulation reliably and fast. However, the continuous reformulations RCCF-ε-opt and RCCF-pen also perform well if solved with KNITRO. Regarding the local solvers, the main outcome is that the specific formulation of the model is crucial for the applied solvers. Note that, by using GAMS, all solvers solve exactly the same model but the results are very heterogeneous among the solvers.

4.2.2. *Type-2 Instances.* For the type-2 instances, for which no binary solution is guaranteed, no BC-MCP solution is found for any of the randomly generated instances. One possible reason is that, by construction of the instances, there simply exist no BC-MCP, i.e., binary-feasible, solution. Thus, both the mixed-integer BC-MCP as well as the CCF model cannot yield a feasible solution and we hence exclude them from the following discussions. In contrast, we can compute approximate solutions using the RCCF-ε, RCCF-ε-opt, and RCCF-pen models. For the RCCF-ε-opt and RCCF-pen formulations, we then obtain a continuous solution minimizing the ℓ_∞- and ℓ_1-norm distances, respectively, to a BC-MCP solution (if the model is solved to global optimality).

Tables 7–10 contain the numerical results obtained for the second type of randomly generated test problems in a similar way to the tables discussed in the last section. However, we include the information about the average objective values, i.e., the average distances of the approximate solutions to a binary feasible point, for the RCCF-ε-opt and RCCF-pen formulations ("Average") instead of the number of binary solution. Again, this average value is computed based only on those instances that are solved at all.

We can see that with the RCCF-ε-opt and RCCF-pen approaches, using KNITRO, we find local solutions for all smaller instances and for all but one instance for the larger instances. Moreover, the solutions are found pretty fast. For instance, the average computational time for finding a solution with KNITRO is 35.65 seconds for RCCF-ε-opt and 51.56 seconds for RCCF-pen in the case of $n_x = n_y = 700$ and $\rho = 0.15$; see Table 9. In these cases, the average ℓ_∞-distance of a local solution to a BC-MCP solution is at its maximum 0.25 on average and the ℓ_1-distance is 115.99. When the density of the matrix M is increased to $\rho = 0.25$ (Table 8), also SNOPT reported local solutions for almost all of the instances for the RCCF-ε, RCCF-ε-opt, and RCCF-pen models. For example, for the instances with $n_x = n_y = 500$ and $\rho = 0.25$, SNOPT requires 14.06, 19.36, and 22.61 seconds to find a solution using the RCCF-ε, RCCF-ε-opt, and RCCF-pen formulations, respectively. In general, the RCCF-ε formulation is not competitive with the other two types of continuous models in terms of the number of obtained approximate solutions.

Table 7. Numerical results for random instances type 2, $n_x = 500$, $n_y = 500$, and $\rho = 0.15$

	RCCF-ε		RCCF-ε-opt			RCCF-pen		
Solver	Opt	Time	Opt	Time	Average	Opt	Time	Average
KNITRO	13	15.79	25	12.92	0.25	25	14.21	83.11
CONOPT4	0	—	0	—	—	0	—	—
SNOPT	0	—	0	—	—	0	—	—
Ipopt	0	—	23	31.5	0.25	17	37.43	82.79

Table 8. Numerical results for random instances type 2, $n_x = 500$, $n_y = 500$, and $\rho = 0.25$

	RCCF-ε		RCCF-ε-opt			RCCF-pen		
Solver	Opt	Time	Opt	Time	Average	Opt	Time	Average
KNITRO	16	17.29	25	15.63	0.25	24	15.15	83.35
CONOPT4	0	—	0	—	—	0	—	—
SNOPT	25	14.06	25	19.36	0.25	25	22.61	83.26
Ipopt	0	—	20	25.74	0.25	6	49.39	83.37

Table 9. Numerical results for random instances type 2, $n_x = 700$, $n_y = 700$, and $\rho = 0.15$

	RCCF-ε		RCCF-ε-opt			RCCF-pen		
Solver	Opt	Time	Opt	Time	Average	Opt	Time	Average
KNITRO	17	40.68	24	35.65	0.25	24	51.56	115.99
CONOPT4	0	—	0	—	—	0	—	—
SNOPT	0	—	0	—	—	0	—	—
Ipopt	0	—	23	53.42	0.25	9	58.01	116.14

Table 10. Numerical results for random instances type 2, $n_x = 700$, $n_y = 700$, and $\rho = 0.25$

	RCCF-ε		RCCF-ε-opt			RCCF-pen		
Solver	Opt	Time	Opt	Time	Average	Opt	Time	Average
KNITRO	15	32.22	24	33.04	0.25	24	47.72	116.05
CONOPT4	0	—	0	—	—	0	—	—
SNOPT	23	32.15	19	41.36	0.25	25	68.98	116.11
Ipopt	0	—	23	50.83	0.25	8	53.8	116.32

To summarize, the continuous reformulations, especially the RCCF-ε-opt and RCCF-pen models can be used to compute an approximate BC-MCP solution in the case when it is known that no exact solution exists.

4.3. **Numerical Results for Spatial Price Equilibrium Instances.** We generated 25 instances for each size and each configuration of δ_i and γ values. As presented in Section 3.2, the sizes considered are 20 supply points and 40 demand points in the first case as well as 25 supply points and 50 demand points in the second case. This leads to 20 binary and 800 continuous variables as well as 25 binary and 1250 continuous variables, respectively; see Table 1. The values of δ_i are generated as follows: First, the 25 SPE instances are solved without any if-then conditions. By construction, a solution always exists in this case; see Section 3.2. Second, we compute the 20 and 30 percentiles p_{20} and p_{30} of the total flow of the 25 instances. Finally, each δ_i was generated randomly in the interval $[p_{20}, p_{30}]$. The fraction γ of the total flow ensured if the contractual minimum δ_i is not reached is set to $1/(8|I|)$ and $1/(25|I|)$.

We start by discussing the results for the SPE with linear transportation costs (Section 4.3.1) and afterward proceed with the results for SPEs with quadratic costs (Section 4.3.2).

4.3.1. *Linear Transportation Costs.* In Tables 11–15, we report the results obtained for the SPE instances with linear transportation costs, with if-then logic constraints and the different combinations of model formulation and solver. The structure of the tables are the same as in the last sections. As mentioned before, the existence of solutions for the SPE instances is not guaranteed if equity-enforcing constraints are added. Hence, the number of instances in which a BC-MCP solution exists is not known a priori.

We observe that for these instances, the RCCF-ε-opt and RCCF-pen approaches always perform better than the original BC-MCP formulation. To be more specific, using the RCCF-ε-opt or RCCF-pen models and local solvers, (i) more instances are solved to a BC-MCP solution compared to the BC-MCP formulation solved with global solvers or (ii) the same number of instances is solved but with less computation time. For example, we can see in Table 11, that for 20 demand and 40 supply points as well as $\gamma = 1/(25|I|)$, 16 instances are solved with an average running time of 94.8 seconds using the BC-MCP formulation and KNITRO. However, the same 16 instances are solved (also obtaining a binary-feasible solution) by applying Ipopt to the RCCF-ε-opt formulation and only 27.56 seconds are required; see Table 13.

Moreover, for $|I| = 25$ and $|J| = 50$ and $\gamma = 1/(25|I|)$, the BC-MCP formulation solves 11 out of 25 instances (Table 11), whereas 19 or 18 instances can be solved in shorter time to a BC-MCP solution if the RCCF-ε-opt and RCCF-pen models are used, respectively; see Table 15. Furthermore, it can been seen in Tables 12–15 that for the instances in which a BC-MCP solution is not obtained, the RCCF-ε, RCCF-ε-opt and RCCF-pen reformulations always find a local solution with at least one of the applicable solvers. In this case, KNITRO seems to be the best solver for the BC-MCP formulation, and Ipopt the best one for the RCCF-ε-opt and RCCF-pen reformulations.

The CCF and RCCF-ε formulations did not perform well for these test problems since only very few BC-MCP solutions can be found using these continuous reformulations. For example, Table 12 shows that using CCF and RCCF-ε, we find BC-MCP solution for 3 and 0 instances, respectively, whereas using the RCCF-ε-opt and RCCF-pen formulations, we find 9 and 11 BC-MCP solutions, respectively.

Finally, it should be noted that SNOPT is not able to solve a single instance of the SPE test set.

In conclusion, the numerical results for the binary-constrained SPE instances with linear transportation costs reveal a clear advantage—both in terms of solution quality and running times—of the RCCF-ε-opt and RCCF-pen reformulations. Using these two continuous reformulations we obtain, in most of the cases, BC-MCP solutions for a larger number of instances or for the same number of instances but with faster running times. A closer look revealed that all solutions are obtained faster except for those cases in which the global solvers can find a solution during their preprocessing or directly at the root node. Moreover, in the cases in which

TABLE 11. Numerical results for thew SPE instances with equity enforcement constraints and linear transportation costs; with $\delta_i \in [p_{20}, p_{30}]$ for the BC-MCP formulation

	$\|I\| = 20,\ \|J\| = 40$				$\|I\| = 25,\ \|J\| = 50$			
	$\gamma = 1/(8\|I\|)$		$\gamma = 1/(25\|I\|)$		$\gamma = 1/(8\|I\|)$		$\gamma = 1/(25\|I\|)$	
Solver	Opt	Time	Opt	Time	Opt	Time	Opt	Time
BARON	3	15.98	5	101.37	0	—	0	—
SCIP	0	—	0	—	0	—	0	—
ANTIGONE	1	50.12	1	53.92	0	—	0	—
KNITRO	11	90.55	16	94.8	3	237.65	11	209.04

TABLE 12. Numerical results for the SPE instances with equity enforcement constraints and linear transportation costs; with $|I| = 20$, $|J| = 40$, $\delta_i \in [p_{20}, p_{30}]$, $\gamma = 1/(8|I|)$

	CCF		**RCCF-ε**			**RCCF-ε-opt**			**RCCF-pen**		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	3	96.45	9	0	83.57	9	3	100.62	15	6	107.37
CONOPT4	2	37.39	25	0	9.64	25	1	9.19	25	1	9.46
SNOPT	0	—	0	0	—	0	0	—	0	0	—
Ipopt	1	3.45	25	0	11.99	25	9	26.7	25	11	57.61

TABLE 13. Numerical results for the SPE instances with equity enforcement constraints and linear transportation costs; with $|I| = 20$, $|J| = 40$, $\delta_i \in [p_{20}, p_{30}]$, $\gamma = 1/(25|I|)$

	CCF		**RCCF-ε**			**RCCF-ε-opt**			**RCCF-pen**		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	3	71.33	10	0	68.21	6	5	109.47	17	11	122.95
CONOPT4	2	40.9	25	0	9.36	25	1	9.02	25	1	9.55
SNOPT	0	—	0	0	—	0	0	—	0	0	—
Ipopt	1	3.76	25	0	15.02	25	16	27.56	25	16	53.19

a binary solution could not be found with any of the proposed formulation (for instance because there might exist no binary-feasible solution), the RCCF-ε-opt and RCCF-pen can be used to compute approximate solutions that minimize the ℓ_∞- or ℓ_1-norm distance, respectively, to a binary solution.

4.3.2. *Quadratic Transportation Costs.* Following the same structure as for the case of linear transportation costs, we report in Tables 16–20 the results collected for the SPE instances with quadratic transportation costs and if-then logic constraints for the different combinations of formulations and solvers. In the quadratic case, the number of instances for which a BC-MCP solution exists is not known a priori as well.

For these type of instances of the SPE, the continuous reformulations again seem to perform better than the BC-MCP formulation in terms of finding BC-MCP solutions for a larger number of instances. For example, we can see in Table 18, that for 20 demand and 40 supply points as well as $\gamma = 1/(25|I|)$, 16 instances

TABLE 14. Numerical results for the SPE instances with equity enforcement constraints and linear transportation costs; with $|I| = 25$, $|J| = 50$, $\delta_i \in [p_{20}, p_{30}]$, $\gamma = 1/(8|I|)$

	CCF		RCCF-ε			RCCF-ε-opt			RCCF-pen		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	2	207.29	11	0	166.98	4	1	85.07	12	5	167.83
CONOPT4	0	—	25	0	51.78	25	0	56.06	25	0	50.04
SNOPT	0	—	0	0	—	0	0	—	0	0	—
Ipopt	0	—	25	0	79.32	25	6	134.94	4	1	218.52

TABLE 15. Numerical results for the SPE instances with equity enforcement constraints and linear transportation costs; with $|I| = 25$, $|J| = 50$, $\delta_i \in [p_{20}, p_{30}]$, $\gamma = 1/(25|I|)$

	CCF		RCCF-ε			RCCF-ε-opt			RCCF-pen		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	8	191.3	14	0	150.93	2	2	10.73	11	10	153.24
CONOPT4	0	—	25	0	45.22	25	0	48.42	25	0	45.86
SNOPT	0	—	0	0	—	0	0	—	0	0	—
Ipopt	1	24.3	25	0	49.03	25	19	75.03	24	18	219.05

are solved (reporting a BC-MCP solution) with the RCCF-pen reformulation and Ipopt solver; meanwhile with the BC-MCP formulation, 15 instances are solved using solver BARON; see Table 16.

Furthermore, in Table 20, for $|I| = 25$, $|J| = 50$ and $\gamma = 1/(25|I|)$, the RCCF-ε formulation finds a BC-MCP solution for 8 out of the 25 instances using CONOPT4, whereas the BC-MCP formulation finds a binary solution for 6 of the instances with BARON solver (Table 16).

Regarding CPU times, there is not a clear winner. For instance, in the case of $|I| = 25$, $|J| = 50$, and $\gamma = 1/(8|I|)$, the number of instances solved with a BC-MCP solution (7 out of 25) is the same for the BC-MCP formulation with BARON and for the RCCF-pen formulation solved with CONOPT4; see Tables 16 and 19. The average running time is around 200 seconds in both cases.

However, there exist one configuration (out of four) of parameters for which the BC-MCP formulation finds more binary solution than the continuous reformulations. This is the case in which 20 demand as well as 40 supply points are considered and the parameter γ is set to $1/(8|I|)$. The BC-MCP formulation finds a binary solution for 16 of the instances using BARON; see Table 16. However, using continuous reformulations, BC-MCP solutions are found for 14 instances with the RCCF-pen reformulation and Ipopt; see Table 17. We can observe in Table 16 that BARON performs rather efficiently for this particular type of instances, finding most of the solutions during preprocessing or at the root node.

Moreover, as it was the case for the SPE instances with linear transportation costs, for those instances for which a BC-MCP solution is not found, the RCCF-ε, RCCF-ε-opt, and RCCF-pen reformulations find, in most of the cases, a local solution with at least one of the applicable solvers; see Tables 17–20. In these cases, CONOPT4 seems to be the best choice.

In conclusion, the numerical results presented in this section reveal the tendency that using the studied continuous reformulations it is possible to find a BC-MCP solution for a larger, or at least for the same, number of instances than with using

Table 16. Numerical results for the SPE instances with equity enforcement constraints and quadratic transportation costs; with $\delta_i \in [p_{20}, p_{30}]$ for the BC-MCP formulation

	$\|I\| = 20,\ \|J\| = 40$				$\|I\| = 25,\ \|J\| = 50$			
	$\gamma = 1/(8\|I\|)$		$\gamma = 1/(25\|I\|)$		$\gamma = 1/(8\|I\|)$		$\gamma = 1/(25\|I\|)$	
Solver	Opt	Time	Opt	Time	Opt	Time	Opt	Time
BARON	16	80.38	15	65.07	7	201.95	6	202.89
SCIP	0	—	0	—	0	—	0	—
ANTIGONE	0	—	1	36.85	0	—	0	—
KNITRO	4	244.78	7	224.62	1	270.57	0	—

Table 17. Numerical results for the SPE instances with equity enforcement constraints and quadratic transportation costs; with $|I| = 20$, $|J| = 40$, $\delta_i \in [p_{20}, p_{30}]$, $\gamma = 1/(8|I|)$

	CCF		**RCCF-ε**			**RCCF-ε-opt**			**RCCF-pen**		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	3	203.73	1	0	240.66	14	6	226.95	9	6	239.06
CONOPT4	4	78.27	25	4	67.58	25	4	66.93	25	4	69.22
SNOPT	0	—	1	0	83.83	1	0	69.44	0	0	—
Ipopt	4	119.89	14	0	99.51	15	12	162.69	16	14	131.96

Table 18. Numerical results for the SPE instances with equity enforcement constraints and quadratic transportation costs; with $|I| = 20$, $|J| = 40$, $\delta_i \in [p_{20}, p_{30}]$, $\gamma = 1/(25|I|)$

	CCF		**RCCF-ε**			**RCCF-ε-opt**			**RCCF-pen**		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	1	197.16	5	0	207.27	16	8	165.06	9	6	218.29
CONOPT4	5	103.06	25	4	67.28	25	4	66.19	25	4	62.95
SNOPT	0	—	0	0	—	2	0	43.68	0	0	—
Ipopt	4	117.93	18	0	134.45	15	12	152.53	18	16	131.05

the BC-MCP formulation. However, the results discussed for the quadratic cost functions are not as pronounced as for the linear case. Nevertheless, for most of the instances for which a BC-MCP solution is not found (for instance because there might exist no binary-feasible solution), the RCCF-ε-opt, RCCF-pen, and RCCF-ε reformulations lead to a locally optimal solution, minimizing the ℓ_∞- or ℓ_1-norm distance to a binary solution.

5. Conclusion

In this paper, we presented different continuous reformulations of the binary-constrained mixed complementarity problem. The main idea is to obtain purely continuous reformulations so that local NLP solvers can be applied that are usually faster compared to mixed-integer solvers. This comes at the price that one only obtains local solutions. An additional advantage of the proposed continuous reformulations is that—in the case that no binary-feasible equilibrium exists—we prove that the approximated solutions that we deliver minimize the violation of

Table 19. Numerical results for the SPE instances with equity enforcement constraints and quadratic transportation costs; with $|I| = 25$, $|J| = 50$, $\delta_i \in [p_{20}, p_{30}]$, $\gamma = 1/(8|I|)$

	CCF		**RCCF-ε**			**RCCF-ε-opt**			**RCCF-pen**		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	2	28.07	0	0	-	1	1	290.95	0	0	-
CONOPT4	5	273.34	17	5	209.37	13	5	213.24	19	7	202.49
SNOPT	0	—	0	0	—	0	0	—	0	0	—
Ipopt	4	272.96	5	0	239.05	1	1	289.3	1	0	243.1

Table 20. Numerical results for the SPE instances with equity enforcement constraints and quadratic transportation costs; with $|I| = 25$, $|J| = 50$, $\delta_i \in [p_{20}, p_{30}]$, $\gamma = 1/(25|I|)$

	CCF		**RCCF-ε**			**RCCF-ε-opt**			**RCCF-pen**		
Solver	Opt	Time	Opt	BF	Time	Opt	BF	Time	Opt	BF	Time
KNITRO	2	186.84	1	0	219.55	1	0	286.27	0	0	—
CONOPT4	5	234.6	22	8	166.32	16	6	216.28	18	6	222.7
SNOPT	0	—	0	0	—	0	0	—	0	0	—
Ipopt	5	239.4	7	0	194.31	3	3	260.99	1	1	168.98

both complementarity and binary constraints. Moreover, the presented numerical results reveal that our approach is performing well both in terms of solution times and solution quality. For the tested binary-constrained spatial price equilibrium problems, the continuous reformulations even outperform the original formulation both in terms of running times and solution quality significantly.

The area of discretely-constrained complementarity problems is a rather young field of research. Thus, many open questions are left for future research. Regarding algorithms, the development of tailored global solution methods for this problem class would be valuable. Within these global approaches, the continuous reformulations studied in this paper can then be used as primal heuristics. Finally, by introducing additional complementarity constraints to model binary variables, the resulting system is not square anymore. Another direction of future research might thus be to theoretically analyze such non-square complementarity problems.

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Appendix A. Big-Ms for the Spatial Price Equilibrium Problem

In this section, we derive correct values for the big-Ms used in Constraints (13a) and (13b) in Section 3.2. We start with M_i in Constraints (13a). Since the supply functions have positive intercept and are monotonically increasing, we have

$$\Psi_i\left(\sum_{j\in J} x_{ij}\right) = \rho_i \sum_{j\in J} x_{ij} + \gamma_i \geq 0$$

for all $x_{ij} \geq 0$, which directly leads to

$$-\sum_{j\in J} x_{ij} \leq \frac{\gamma_i}{\rho_i}.$$

Note that $\rho_i > 0$ holds. Thus, $M_i = \delta_i + \gamma_i/\rho_i$ is a valid choice.

Again using the assumptions stated in Section 3.2, the SPE problem (12) is equivalent to the Karush–Kuhn–Tucker conditions of the following optimization problem; cf., e.g., [11, 39]:

$$\min_{s,d,x} \quad \sum_{i \in I} \int_0^{s_i} \Psi_i(\tau) \, \mathrm{d}\tau + \sum_{i \in I} \sum_{j \in J} \int_0^{x_{ij}} c(\tau) \, \mathrm{d}\tau - \sum_{j \in J} \int_0^{d_j} \theta_j(\tau) \, \mathrm{d}\tau \tag{14a}$$

$$\text{s.t.} \quad \sum_{j \in J} x_{ij} = s_i, \quad i \in I, \tag{14b}$$

$$\sum_{i \in I} x_{ij} = d_j, \quad j \in J, \tag{14c}$$

$$x_{i,j} \geq 0, \quad i \in I, \ j \in J. \tag{14d}$$

This can be seen as the problem of a central planner who simultaneously decides on all supplies $s = (s_i)_{i \in I}$, all demands $d = (d_j)_{j \in J}$, and all flows $x = (x_{ij})_{(i,j) \in A}$. Moreover, it is easy to verify that this optimization problem is equivalent to the setting in which all suppliers, consumers, and the transporting company solve separate optimization problems that are equilibrated using the market clearing conditions (14b) and (14c). In this setting, the problem of consumer $j \in J$ is given by

$$\max_{d_j} \quad \int_0^{d_j} \theta_j(\tau) \, \mathrm{d}\tau - \rho_j d_j.$$

Thus, by optimality, we obtain

$$\theta_j(d_j) = \theta_j \left(\sum_{i \in I} x_{ij} \right) = -\rho_j' \sum_{i \in I} x_{ij} + \gamma_j' \geq 0$$

in an equilibrium. Hence,

$$\sum_{i \in I} x_{ij} \leq \frac{\gamma_j'}{\rho_j'} \quad \text{for all } j \in J$$

and

$$M_i' = \frac{\gamma_i}{\rho_i} + \gamma \sum_{j \in J} \frac{\gamma_j'}{\rho_j'}$$

is a valid choice.

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