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Cycles and global attractors of reactantless and inhibitorless reaction systems

Rocco Ascone [a,*], Giulia Bernardini [a,b], Luca Manzoni [a]

[a] *University of Trieste, Italy*
[b] *University of Milan, Italy*

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ABSTRACT

We explore the computational complexity of deciding the existence of fixed points and cycles that can be reached from any other states (called *global attractors*) in the dynamics of inhibitorless and reactantless reaction systems. The problems we consider are all known to be **PSPACE**-complete in the case of unconstrained reaction systems; in this paper, we show that some of them become polynomially solvable when limited to inhibitorless and reactantless reaction systems, while others remain **PSPACE**-complete. Specifically, we prove that the problems of deciding (i) if a given state belongs to a cycle, (ii) whether two reaction systems have at least one cycle in common, and (iii) whether they have the same set of cycles, remain **PSPACE**-complete even in the inhibitorless and reactantless classes, as well as the problem of deciding if a global cycle attractor exists in a reactantless reaction system. Interestingly, however, we demonstrate that no global cycle attractor of length at least 2 can exist in inhibitorless reaction systems; and no global cycle attractor of length greater than 2 can exist in reactantless reaction systems. Furthermore, we show that the problems of deciding whether a given state is a global attractor and whether a global fixed point attractor exists become polynomially solvable when restricted to inhibitorless and reactantless reaction systems.

1. Introduction

Introduced nearly two decades ago by Ehrenfeucht and Rozenberg [1], reaction systems are an abstract computational model inspired by the chemical reactions occurring in living cells. The notion at the heart of this model is that the biochemical processes within a cell can be simulated using a limited collection of entities that represent various substances, alongside a set of rules that mimic reactions. A reaction is characterized by its reactants, inhibitors, and products, and it occurs when the set of entities currently present in the cell (i.e. the system's state) includes all reactants and lacks any inhibitors, resulting in the reaction's products.

Whenever a set of reactions occurs in a certain state, the system's subsequent state is determined by the union of the products of all those reactions. This process defines a dynamical system whose points are given by all the possible subsets of entities, i.e. all possible states of the reaction system. Determining the computational complexity of deciding the occurrence of various behaviours of such dynamical systems has been the object of a great deal of research work [2–8].

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* Corresponding author.
E-mail addresses: rocco.ascone@phd.units.it (R. Ascone), giulia.bernardini@units.it (G. Bernardini), lmanzoni@units.it (L. Manzoni).

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Table 1
Computational complexity of the problems studied in this work for different classes of reaction systems. $\mathcal{RS}(\infty,\infty)$, $\mathcal{RS}(0,\infty)$ and $\mathcal{RS}(\infty,0)$ denote unconstrained, reactantless and inhibitorless reaction systems, respectively (see Definition 1). Light-blue cells contain the results proved in this paper. (For interpretation of the colours in the table, the reader is referred to the web version of this article.)

Problem		$\mathcal{RS}(\infty,\infty)$	$\mathcal{RS}(0,\infty)$	$\mathcal{RS}(\infty,0)$
A given state is a global attractor		**PSPACE**-c [33]	**P** (Corollary 25)	**P** (Corollary 5)
∃ global fixed point attractor		**PSPACE**-c [33]	**P** (Corollary 26)	**P** (Corollary 6)
∃ global cycle attractor of length at least k	$k = 2$	**PSPACE**-c [7]	**PSPACE**-c (Theorem 30)	$\nexists$ (Lemma 7)
	$k > 2$	**PSPACE**-c [7]	$\nexists$ (Proposition 27)	$\nexists$ (Lemma 7)
A given state is part of a cycle		**PSPACE**-c [33]	**PSPACE**-c (Corollary 34)	**PSPACE**-c (Theorem 20)
∃ common cycle		**PSPACE**-c [33]	**PSPACE**-c (Theorem 35)	**PSPACE**-c (Theorem 22)
sharing all cycles		**PSPACE**-c [33]	**PSPACE**-c (Theorem 35)	**PSPACE**-c (Theorem 21)

Reaction systems operate on a qualitative basis, meaning that the presence of a reactant in a given state implies it is available in sufficient quantities for all reactions that require it, thus avoiding conflicts over shared resources. Other related models waiving this assumption have been proposed in the literature, see e.g. [9–18]. Nevertheless, the computational power of the simpler qualitative model has been demonstrated by several studies [19–25] showing that reaction systems can be effectively used to simulate various biological processes.

Although the conventional framework for reaction systems does not limit the number of reactants and inhibitors involved in each reaction, an alternative branch of research concentrates on systems with constrained resources. Ehrenfeucht et al. [26] first investigated how bounding the number of reactants and inhibitors in the reactions can affect the kinds of functions that a reaction system can define. Manzoni et al. [27] then classified resource-bounded systems in such a way that the reaction functions enjoy specific properties within each class: in particular, they identified the class of *inhibitorless* reaction systems, in which all reactions have an empty set of inhibitors; the class of *reactantless* systems in which the set of reactants is always empty; and the class of reaction systems, later named *additive* [28], in which each reaction only uses one reactant and no inhibitors.

Dennunzio et al. [29] studied the complexity of reachability in several subclasses of inhibitorless and reactantless systems; Azimi et al. [30] studied how to list all steady states of a system whose reactions have a small quantity of both reactants and inhibitors; Teh et al. [31] studied the evolvability problem in reactantless and inhibitorless systems; and Ascone et al. investigated the computational complexity of problems related to the existence of fixed points and attractors in reactantless and inhibitorless systems [32] and in additive systems [28].

Contributions In this paper, we study the computational complexity of deciding on the existence of fixed points and cycles that are also *global attractors* (i.e. they can be reached from every other state) in inhibitorless and reactantless reaction systems. All these problems were shown to be **PSPACE**-complete in unconstrained reaction systems [33]. Interestingly, we show that disabling either the set of reactants or the set of inhibitors reduces to polynomial the complexity of deciding whether a global fixed point attractor exists and if a given state is a global attractor. Furthermore, we prove that only trivial cycles consisting of a single state can exist in the dynamics of inhibitorless systems, while in reactantless systems cycles of two states may occur, and it is **PSPACE**-complete to decide on their existence. Finally, we prove that the problems deciding whether a given state belongs to some cycle, whether two reaction systems have at least one cycle in common, and whether two reaction systems have the same set of cycles remain **PSPACE**-complete even in the reactantless and inhibitorless cases. Table 1 summarizes our results.

2. Basics notions

Given a finite set S of *entities*, a *reaction* a over S is a triple (R_a, I_a, P_a) of subsets of S; R_a is the set of *reactants*, I_a the set of *inhibitors*, and P_a the nonempty set of *products*. In this paper, the reactants and inhibitors of a reaction are allowed to be empty sets as in the original definition of reaction systems [1]. The set of all reactions over S is denoted by $\mathrm{rac}(S)$. A *reaction system* (RS) $\mathcal{A} = (S, A)$ where S consists of the finite set of entities S, called the *background set*, and a set $A \subseteq \mathrm{rac}(S)$ of reactions over S.

Any subset of S is a *state* of the reaction system; a reaction a is *enabled* in a state T when $R_a \subseteq T$ and $I_a \cap T = \emptyset$, and the set of all the reactions of $\mathcal{A}$ enabled in T is denoted by $\mathrm{en}_{\mathcal{A}}(T)$. The *result function* $\mathrm{res}_a : 2^S \to 2^S$ of a reaction a, where 2^S denotes the power set of S, is defined as

$$\mathrm{res}_a(T) := \begin{cases} P_a & \text{if } a \text{ is enabled in } T \\ \emptyset & \text{otherwise.} \end{cases}$$

The definition of res_a naturally extends to sets of reactions: given any $T \subseteq S$ and $A \subseteq \mathrm{rac}(S)$, we define $\mathrm{res}_A(T) := \bigcup_{a \in A} \mathrm{res}_a(T)$. Consistently, the result function $\mathrm{res}_{\mathcal{A}}$ of the whole RS $\mathcal{A} = (S, A)$ is defined to be equal to res_A, i.e. the result function of the whole set of reactions of the reaction system. In this way, any RS $\mathcal{A} = (S, A)$ induces a discrete dynamical system with state set 2^S and next state function $\mathrm{res}_{\mathcal{A}}$.

In this paper, we are interested in the dynamics of RS, that is, the study of the successive states of the system under the action of the result function $\mathrm{res}_{\mathcal{A}}$ starting from some initial set of entities. The *orbit* or *state sequence* of a given state T of a RS $\mathcal{A}$ is defined as the sequence of states obtained by subsequent iterations of $\mathrm{res}_{\mathcal{A}}$ starting from T, namely, the sequence $(T, \mathrm{res}_{\mathcal{A}}(T), \mathrm{res}^2_{\mathcal{A}}(T), \dots)$.

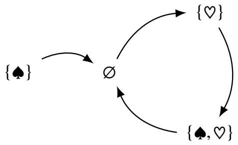

Fig. 1. A global 3-cycle attractor in the dynamics of the RS $\mathcal{A} = (S, A)$ with background set $S = \{♠, ♡\}$ and reactions $A = \{(\varnothing, \{♠, ♡\}, \{♡\}), (\{♡\}, \{♠\}, \{♠, ♡\})\}$. Arrows connect each state T with $\mathrm{res}_{\mathcal{A}}(T)$.

(a) Dynamics of the reactantless RS given by the reaction $(\varnothing, \{♠, ♡\}, \{♠\})$.

(b) Dynamics of the inhibitorless RS given by the reaction $(\{♠\}, \varnothing, \{♠, ♡\})$.

Fig. 2. A global 2-cycle attractor (2a) and a global attractor consisting of two fixed points (2b). No global 3-cycle attractor (like the one in Fig. 1) can exist in the dynamics of reactantless RS (Lemma 7) or in the dynamics of inhibitorless RS (Proposition 27).

Table 2
Functions computed by several classes of RS.

Class of RS	Subclass of $2^S \to 2^S$
$\mathcal{RS}(\infty, \infty)$	all
$\mathcal{RS}(0, \infty)$	antitone
$\mathcal{RS}(\infty, 0)$	monotone
$\mathcal{RS}(1, 0)$	additive
$\mathcal{RS}(0, 0)$	constant

Note that since S is finite, for any state T the sequence $\left(\mathrm{res}^n_{\mathcal{A}}(T)\right)_{n\in\mathbb{N}}$ is always ultimately periodic. In particular, the orbit of a state T is a *cycle* of length k (or k-cycle) if there exists $k \in \mathbb{N}$ such that $\mathrm{res}^k_{\mathcal{A}}(T) = T$, and $\mathrm{res}^h_{\mathcal{A}}(T) \neq T$ for every $h < k$. In the special case where $k = 1$, T is said to be a *fixed point*.

Any set of cycles forms an *invariant set* for $\mathcal{A}$: a set of states $\mathcal{U} \subseteq 2^S$ such that $\cup_{U\in\mathcal{U}}\{\mathrm{res}_{\mathcal{A}}(U)\} = \mathcal{U}$. Conversely, any invariant set for $\mathcal{A}$ is a set of cycles [33]. A *local attractor* for $\mathcal{A}$ is an invariant set $\mathcal{U}$ such that there exists an external state $T \notin \mathcal{U}$ with $\mathrm{res}_{\mathcal{A}}(T) \in \mathcal{U}$. An invariant set $\mathcal{U}$ is a *global attractor* if for all states $T \in 2^S$ there exists $k \in \mathbb{N}$ such that $\mathrm{res}^k_{\mathcal{A}}(T) \in \mathcal{U}$, i.e. $\mathcal{U}$ is eventually reached from every possible state of $\mathcal{A}$. When a global attractor $\mathcal{U}$ consists of only one state T, we say that T is a *global fixed-point attractor*. Similarly, $\mathcal{U}$ is a *global cycle attractor* if all the states in $\mathcal{U}$ belong to the same cycle (see Fig. 1 for an example).

We now recall the classification of reaction systems in terms of the number of resources employed per reaction [27].

Definition 1 *([27]).* Let $i, r \in \mathbb{N}$. The class $\mathcal{RS}(r, i)$ consists of all RS having at most r reactants and i inhibitors for each reaction. We also define the (partially) unbounded classes $\mathcal{RS}(\infty, i) = \bigcup_{r=0}^{\infty} \mathcal{RS}(r, i)$, $\mathcal{RS}(r, \infty) = \bigcup_{i=0}^{\infty} \mathcal{RS}(r, i)$, and $\mathcal{RS}(\infty, \infty) = \bigcup_{r=0}^{\infty} \bigcup_{i=0}^{\infty} \mathcal{RS}(r, i)$.

We will call $\mathcal{RS}(0, \infty)$ the class of *reactantless* systems, and $\mathcal{RS}(\infty, 0)$ the class of *inhibitorless* systems. See Fig. 2 for an example of a reactantless RS and an inhibitorless RS.

The classification of Definition 1 does not consider the number of products as a parameter because RS can always be assumed to be in *singleton product normal form* [34]: any reaction $(R, I, \{p_1, \ldots, p_m\})$ can be replaced by the set of reactions $(R, I, \{p_1\}), \ldots, (R, I, \{p_m\})$ that produce the same result.

Five equivalence classes of RS implied by Definition 1 have a characterisation in terms of functions over the Boolean lattice 2^S [27], listed in Table 2. Recall that a function $f : 2^S \to 2^S$ is *antitone* if $X \subseteq Y$ implies $f(X) \supseteq f(Y)$, *monotone* if $X \subseteq Y$ implies $f(X) \subseteq f(Y)$, *additive* (or an upper-semilattice endomorphism) if $f(X \cup Y) = f(X) \cup f(Y)$ for all $X, Y \in 2^S$. We say that the RS $\mathcal{A} = (S, A)$ computes the function $f : 2^S \to 2^S$ if $\mathrm{res}_{\mathcal{A}} = f$.

3. Global attractors of inhibitorless reaction systems

In this section, we study the complexity of deciding the existence of a global fixed-point attractor or a global cycle attractor in inhibitorless reaction systems.

3.1. Existence of a global fixed-point attractor

We begin with a simple observation that immediately follows from the definition of global fixed-point attractors.

Observation 2. A reaction system with a global fixed-point attractor cannot have any other fixed points or cycles.

In particular, Observation 2 implies that if a global fixed-point attractor exists, it is unique. Proposition 3 characterizes global fixed-point attractors for monotone functions.

Proposition 3. *Let S be a finite set of n elements, $f : 2^S \to 2^S$ a monotone function and T a fixed point for f consisting of t elements. Then, T is a global fixed-point attractor for f if and only if $f^t(\varnothing) = T = f^{n-t}(S)$.*

Proof. $\boxed{\Rightarrow}$ Consider the sequence $\varnothing \subsetneq f(\varnothing) \subsetneq \cdots \subsetneq f^m(\varnothing) = f^{m+1}(\varnothing)$: we have $|f^m(\varnothing)| \geq m$. If it held $f^m(\varnothing) \subsetneq T$, a fixed point would exist different from T, and therefore, T would not be a global attractor by Observation 2. Thus it must be $f^m(\varnothing) = T$; since $t = |T| = |f^m(\varnothing)| \geq m$, from the monotonicity of f we derive the following facts:

$$\varnothing \subseteq f^{t-m}(\varnothing) \Rightarrow f^m(\varnothing) \subseteq f^t(\varnothing);$$

$$\varnothing \subseteq T \Rightarrow f^t(\varnothing) \subseteq f^t(T).$$

Collecting all together, we obtain $T = f^m(\varnothing) \subseteq f^t(\varnothing) \subseteq f^t(T) = T$, implying that $f^t(\varnothing) = T$. Consider now the sequence $S \supsetneq f(S) \supsetneq \cdots \supsetneq f^k(S) = f^{k+1}(S)$: we have $|f^k(S)| \leq n-k$. If it held $f^k(S) \supsetneq T$, then there would exist a fixed point different from T, and therefore, T would not be a global attractor by Observation 2. We obtain that $f^k(S) = T$; since $t = |T| = |f^k(S)| \leq n-k$, from the monotonicity of f we derive the following facts:

$$S \supseteq f^{n-k-t}(S) \Rightarrow f^k(S) \supseteq f^{n-t}(S);$$

$$S \supseteq T \Rightarrow f^{n-t}(S) \supseteq f^{n-t}(T).$$

Collecting all together, we obtain $T = f^k(S) \supseteq f^{n-t}(S) \supseteq f^{n-t}(T) = T$, implying in particular that $f^{n-t}(S) = T$.

$\boxed{\Leftarrow}$ We need to prove that $T = f^t(\varnothing) = f^{n-t}(S)$ is a global attractor. Consider any state $\varnothing \subsetneq T' \subsetneq S$: by monotonicity, it holds that $T = f^t(\varnothing) \subseteq f^t(T')$ and $f^{n-t}(T') \subseteq f^{n-t}(S) = T$. We divide two cases.

Case (i): $t \leq n-t$. Since $T \subseteq f^t(T')$, then it holds $f^{n-2t}(T) \subseteq f^{n-2t+t}(T') \Rightarrow T \subseteq f^{n-t}(T') \subseteq T$, and therefore T' reaches T in at most $n-t$ steps.

Case (ii): $t > n-t$. Since $T \supseteq f^{n-t}(T')$, then $f^{2t-n}(T) \supseteq f^{2t-n+n-t}(T') \Rightarrow T \supseteq f^t(T') \supseteq T$, therefore T' reaches T in at most t steps. □

Proposition 3 immediately gives a criterion for deciding the existence of a global fixed-point attractor for monotone functions, formalised in Corollary 4.

Corollary 4. *Given S a finite set of n elements, and $f : 2^S \to 2^S$ monotone, there exists a global fixed-point attractor if and only if $f^t(\varnothing) = f^{n-t}(S)$ for some $0 \leq t \leq n$.*

Proposition 3 and Corollary 4 can be directly applied to inhibitorless reaction systems, whose result functions are always monotone. We obtain the following results.

Corollary 5. *Given a RS $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ and a state $T \subseteq S$, deciding if T is a global fixed-point attractor of $\mathcal{A}$ is in* **P**.

Proof. Since $\mathrm{res}_{\mathcal{A}}$ is monotone [27], we can apply Proposition 3. Therefore, T is a global attractor for $\mathcal{A}$ if and only if $\mathrm{res}^t_{\mathcal{A}}(\varnothing) = T = \mathrm{res}^{n-t}_{\mathcal{A}}(S)$ where t and n are the cardinalities of T and S, respectively. For any state $U \subseteq S$, $\mathrm{res}_{\mathcal{A}}(U)$ can be computed in polynomial time: it suffices to check which reactions are enabled in U by intersecting their reactants and inhibitors with U, and then take the union of the products of the enabled functions. To decide if T is a global attractor, we only need to evaluate $\mathrm{res}_{\mathcal{A}}$ at most $|S|$ times; thus, the problem is in **P**. □

Corollary 6. *Given a RS $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$, deciding on the existence of a global fixed-point attractor for $\mathcal{A}$ is in* **P**.

Proof. Since $\mathrm{res}_{\mathcal{A}}$ is monotone [27], we can apply Corollary 4: there exists a global attractor for $\mathcal{A}$ if and only if $\mathrm{res}^t_{\mathcal{A}}(\varnothing) = \mathrm{res}^{n-t}_{\mathcal{A}}(S)$ for some $0 \leq t \leq n$, where n is the cardinality of S. We conclude as in Corollary 5. □

3.2. Existence of a global cycle attractor

We start by giving a result that immediately follows from the Knaster-Tarki theorem [35] and excludes the existence of a global cycle attractor of length greater than one in the case of monotone functions. In particular, this implies that no global cycle attractor of length $k \geq 2$ can exist in the dynamics of inhibitorless reaction systems, as their result function is always monotone [27].

Lemma 7. *Let $f : 2^S \to 2^S$ be a monotone function. Then no global k-cycle attractor exists for any $k \geq 2$. Moreover, if $\mathcal{U}$ is a global attractor invariant set, then at least one of the cycles in $\mathcal{U}$ is a fixed point.*

Proof. By the Knaster-Tarki theorem, monotone functions always have a fixed point, therefore a global k-cycle attractor cannot exist for $k > 1$ by Observation 2. For the same reason, if $\mathcal{U}$ is a global attractor invariant set, then at least one of the cycles in $\mathcal{U}$ is a fixed point. ☐

The rest of this section provides results on the existence of global attractors consisting of two fixed points for monotone functions (thus for inhibitorless reaction systems). These results will be useful in Section 5 to prove the complexity of deciding on the existence of global cycle attractors in *reactantless* systems. In Lemma 8, we prove that for any monotone function, a global attractor consisting of two fixed points must have a particular form.

Lemma 8. *Let $f : 2^S \to 2^S$ monotone and $\mathcal{U} = \{T_1, T_2\}$ a global attractor consisting of two fixed points, then $\mathcal{U} = \{f^n(\varnothing), f^m(S)\}$, with $n, m \geq 0$ such that $f^n(\varnothing) = f^{n+1}(\varnothing)$ and $f^m(S) = f^{m+1}(S)$.*

Proof. Let $n, m \geq 0$ such that $f^n(\varnothing) = f^{n+1}(\varnothing)$ and $f^m(S) = f^{m+1}(S)$. By monotonicity, $f^n(\varnothing) \subseteq T_i \subseteq f^m(S)$ for $i = 1, 2$. Suppose towards a contradiction that the inclusions are both strict: then $f^n(\varnothing)$ and $f^m(\varnothing)$ would be fixed points that cannot be attracted by $\mathcal{U}$, a contradiction. We obtain the statement. ☐

Lemma 8 implies that any global attractor consisting of two fixed points in a reaction system $\mathcal{A} \in \mathcal{RS}(\infty, 0)$ must be of the form $\{\mathrm{res}^n_{\mathcal{A}}(\varnothing), \mathrm{res}^m_{\mathcal{A}}(S)\}$. However, this characterization is not strong enough to give a polynomial time algorithm, and in Proposition 9 we prove that, in the special case where $\varnothing$ and S are fixed points, deciding if $\{\mathrm{res}^n_{\mathcal{A}}(\varnothing), \mathrm{res}^m_{\mathcal{A}}(S)\}$ is a global attractor for $\mathcal{A}$ is **coNP**-hard. The proof extends an idea from [32, Theorem 25].

Proposition 9. *Given $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ such that $\varnothing$ and S are fixed points, it is* **coNP***-hard to decide if $\mathcal{U} = \{\varnothing, S\}$ is a global attractor.*

Proof. To show **coNP**-hardness, we reduce VALIDITY [36] to this problem. Given a Boolean formula $\varphi = \varphi_1 \vee \cdots \vee \varphi_m$ in DNF over the variables $V = \{x_1, \ldots, x_n\}$, let $\overline{V} := \{\overline{x_j} : x_j \in V\}$ and $\heartsuit_S := \{\heartsuit_i : 1 \leq i \leq n\}$. We define $\mathrm{pos}(\varphi_r) \subseteq V$ the set of variables that occur non-negated in φ_r and $\overline{\mathrm{neg}}(\varphi_r) \subseteq \overline{V}$ the set of variables that occur negated in φ_r. We then define a RS $\mathcal{A}$ with background set $S := V \cup \overline{V} \cup \heartsuit_S \cup \{\diamond\}$ and reactions

$$(\overline{\mathrm{neg}}(\varphi_j) \cup \mathrm{pos}(\varphi_j) \cup \heartsuit_S, \varnothing, \{\diamond\}) \qquad \text{for } 1 \leq j \leq m \tag{1}$$

$$(\{x_i\} \cup \heartsuit_S, \varnothing, \{\heartsuit_i, x_i\}) \qquad \text{for } 1 \leq i \leq n \tag{2}$$

$$(\{\overline{x_i}\} \cup \heartsuit_S, \varnothing, \{\heartsuit_i, \overline{x_i}\}) \qquad \text{for } 1 \leq i \leq n \tag{3}$$

$$(\{x_i, \overline{x_i}\} \cup \heartsuit_S, \varnothing, \{\diamond\}) \qquad \text{for } 1 \leq i \leq n \tag{4}$$

$$(\{\diamond\} \cup \heartsuit_S, \varnothing, S). \tag{5}$$

Note that $\varnothing$ and S are fixed points; furthermore, any $T \subseteq S$, it falls in one of the following cases:

1) $\heartsuit_S \not\subseteq T$. In this case, $\mathrm{res}_{\mathcal{A}}(T) = \varnothing$, since no reaction is enabled;
2) $\diamond \in T$ and $\heartsuit_S \subseteq T$. In this case, reaction (5) is enabled and thus $\mathrm{res}_{\mathcal{A}}(T) = S$;
3) T is of the form $Y \cup \heartsuit_S$, with $Y \subseteq V \cup \overline{V}$.

Thus $\varnothing$ is reached from any state that does not fully contain $\heartsuit_S$, and S from any state containing both $\heartsuit_S$ and $\diamond$. Let us now focus on the states falling in case (3). For any $Y \subseteq V \cup \overline{V}$, we define $\heartsuit_Y := \{\heartsuit_i : x_i \in Y \vee \overline{x_i} \in Y\} \subseteq \heartsuit_S$. The following subcases can happen:

3.1) $\exists i$ such that both $x_i, \overline{x_i} \in Y$. In this case, the i-th reaction of Group (4) is enabled by $Y \cup \heartsuit_S$, thus $\diamond \in \mathrm{res}_{\mathcal{A}}(Y \cup \heartsuit_S)$; if $\heartsuit_S \subseteq \mathrm{res}_{\mathcal{A}}(Y \cup \heartsuit_S)$ or $\heartsuit_S \not\subseteq \mathrm{res}_{\mathcal{A}}(Y \cup \heartsuit_S)$, then $\mathrm{res}_{\mathcal{A}}(Y \cup \heartsuit_S)$ is either in case (1) or (2) above, implying that $\mathrm{res}^2_{\mathcal{A}}(Y \cup \heartsuit_S) \in \{S, \varnothing\}$;
3.2) $\exists i$ such that both $x_i, \overline{x_i} \notin Y$. Then $\heartsuit_S \not\subseteq \mathrm{res}_{\mathcal{A}}(Y \cup \heartsuit_S)$ since none of the i-th reactions in Groups (2), (3) are enabled, therefore, by case (1), $\mathrm{res}^2(Y \cup \heartsuit_S) = \varnothing$.

3.3) $x_i \in Y \Leftrightarrow \overline{x_i} \notin Y$ for every $1 \le i \le n$. In this case, $Y = X \cup \overline{V \setminus X}$ for some $X \subseteq V$, thus it encodes an assignment for φ where the variables in X are assigned true value and the variables in $V \setminus X$ are assigned value false. Note that being φ in DNF, it is satisfied if and only if at least one φ_i is satisfied; moreover, any clause φ_i, being a conjunction of variables, is satisfied if and only if all of its negated variables are assigned value false and all of its non-negated variables are assigned value true. Therefore, the assignment implied by $X \cup \overline{V \setminus X}$ satisfies φ if and only if $X \cup \overline{V \setminus X} \cup \heartsuit_S$ enables one of the reactions from the Group (1). Hence, if $Y = X \cup \overline{V \setminus X}$ satisfies φ then $\diamondsuit \in \mathrm{res}(Y \cup \heartsuit_S)$, implying $\mathrm{res}^2(Y \cup \heartsuit_S) = S$. If instead Y does not satisfy φ then $\mathrm{res}(Y \cup \heartsuit_S) = Y \cup \heartsuit_S$ by reactions of Groups (2) and (3).

We conclude that $\{\varnothing, S\}$ is a global attractor for $\mathcal{A}$ if and only if all the assignments satisfy φ, i.e. φ is a tautology. Since the mapping $\varphi \mapsto \mathcal{A}$ is computable in polynomial time, the problem is **coNP**-hard. ☐

Note that the proof of Proposition 9 also implies that even the simpler problem of deciding if $\varnothing$ and S are the only fixed points for $\mathcal{A} \in \mathcal{RS}(\infty, 0)$ is **coNP**-complete, as shown in Corollary 10.

Corollary 10. *Given $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ such that $\varnothing$ and S are fixed points, it is* **coNP***-complete to decide if $\varnothing$ and S are the only fixed points.*

Proof. The problem is in **coNP** because there exists a simple non-deterministic algorithm which guesses a state T and then verifies in polynomial time that it is a fixed point different from $\varnothing$ and S. The **coNP**-hardness follows from the same reduction as Proposition 9. ☐

Corollary 10 holds even in the general case, where the fixed points are different from $\varnothing$ and S, as stated in Corollary 11.

Corollary 11. *Let $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ and $\varnothing \subsetneq T_1 \subsetneq T_2 \subsetneq S$ be fixed points such that $T_1 = \mathrm{res}^n_{\mathcal{A}}(\varnothing)$ and $T_2 = \mathrm{res}^m_{\mathcal{A}}(S)$ for some integer $n, m \ge 0$. It is* **coNP***-complete to decide if T_1 and T_2 are the only fixed points.*

Proof. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ such that $\varnothing$ and S are fixed points. We construct $\mathcal{B} = (S', B) \in \mathcal{RS}(\infty, 0)$ where $S' = S \cup \{\heartsuit, \spadesuit\}$ and $B = A \cup \{(\varnothing, \varnothing, \{\heartsuit\})\}$. Since $\mathrm{res}_{\mathcal{A}}(\varnothing) = \varnothing$ and $\mathrm{res}_{\mathcal{A}}(S) = S$, then $\mathrm{res}_{\mathcal{B}}(\{\heartsuit\}) = \{\heartsuit\}$ and $\mathrm{res}_{\mathcal{B}}(S \cup \{\heartsuit\}) = S \cup \{\heartsuit\}$. Furthermore, $\varnothing$ and S are the only fixed points for $\mathcal{A}$ if and only if T_1 and T_2 are the only fixed points for $\mathcal{B}$ with $T_1 = \{\heartsuit\} = \mathrm{res}_{\mathcal{B}}(\varnothing)$, $T_2 = S' \setminus \{\spadesuit\} = \mathrm{res}_{\mathcal{B}}(S')$. ☐

In Section 4 (Theorem 17), we will prove that the problem of deciding if $\{\varnothing, S\}$ is a global attractor is indeed **PSPACE**-complete.

4. Cycles of inhibitorless reaction systems

In this section, we prove **PSPACE**-hardness for problems concerning cycles in the class of inhibitorless reaction systems.

Remark 12. Most of the problems studied in this article were proven to be in **PSPACE** [33] for the general class of all reaction systems $\mathcal{RS}(\infty, \infty)$. In the following, we will thus only focus on the *completeness* of such problems.

Let M be any single-tape deterministic Turing machine using m tape cells during its computation; let Σ be the tape alphabet, Q the set of states, and $\delta : Q \times \Sigma \to Q \times \Sigma \times \{-1, 0, +1\}$ the transition function of M. Following the work in [29], we will define a RS $\mathcal{M} = (S, A) \in \mathcal{RS}(\infty, 0)$ simulating M.
Entities. The set of entities of $\mathcal{M}$ is

$$S := S_\Sigma \cup \heartsuit_\Sigma \cup S_Q \cup \{\diamondsuit_Q\} \cup \{\spadesuit_j : 1 \le j \le m\}$$

where $\heartsuit_\Sigma := \{\heartsuit^j_\Sigma : 1 \le j \le m\}$, $S_\Sigma := \{a_j : a \in \Sigma, 1 \le j \le m\}$ and $S_Q := \{q_j : q \in Q, 1 \le j \le m\}$. The entities have the following meanings:

a_j: the symbol $a \in \Sigma$ is written on cell j;
$\heartsuit^j_\Sigma$: an alphabet symbol is written on cell j;
q_j: the current state is $q \in Q$ and the head is on cell j;
$\spadesuit_j$: the head is not located on cell j;
$\diamondsuit_Q$: a state symbol is present in the configuration.

In this way, the generic configuration where M is in state $q \in Q$, the tape head is on cell i, and the tape contains the string $x = x_1 \cdots x_m$, is encoded as the following state, where $(x_j)_j$ denotes that the symbol x_j on cell j:

$$T = \{(x_j)_j : 1 \le j \le m\} \cup \heartsuit_\Sigma \cup \{q_i, \diamondsuit_Q\} \cup \{\spadesuit_j : 1 \le j \le m, j \ne i\}. \tag{6}$$

We call a state of this form *valid*, in contrast to *invalid* states that do not encode a configuration of M. This construction differs from the one proposed in [29] by the symbols $\heartsuit_\Sigma \cup \{\diamondsuit_Q\}$, which will be used to control the dynamics of $\mathcal{M}$ when the system is in an invalid state.

Example. Consider a Turing machine M working in space $m = 4$ and the configuration where M is in state q, the tape head is located on cell 3, and the tape contains the string *abba*. The state of the RS $\mathcal{M}$ that encodes such a configuration of M is then $T = \{a_1, \heartsuit^1_\Sigma, b_2, \heartsuit^2_\Sigma, b_3, \heartsuit^3_\Sigma, a_4, \heartsuit^4_\Sigma, \spadesuit_1, \spadesuit_2, q_3, \diamondsuit_Q, \spadesuit_4\}$. ⌟

Reactions. Let us denote $\heartsuit := \heartsuit_\Sigma \cup \{\diamondsuit_Q\}$ and $\spadesuit := \{\spadesuit_j : 1 \le j \le m\}$. Each transition $\delta(q, a) = (q', a', d)$ of M, with $q, q' \in Q$, $a, a' \in \Sigma$, and $d \in \{-1, 0, +1\}$, is encoded by the following two sets of reactions:

$$(\{q_i, a_i\} \cup \heartsuit, \emptyset, \{q'_{i+d}, a'_i, \heartsuit^i_\Sigma, \diamondsuit_Q\}) \qquad \text{for } 1 \le i \le m \tag{7}$$

$$(\{q_i, a_i\} \cup \heartsuit, \emptyset, \{\spadesuit_j : 1 \le j \le m, j \ne i + d\}) \qquad \text{for } 1 \le i \le m. \tag{8}$$

If the tape head of M is on cell i, then the i-th reaction from Group (7) produces the entity encoding the new state q' and the new tape head position $i + d$ of M, the symbol written on cell i and the flag symbols $\heartsuit^i_\Sigma, \diamondsuit_Q$; and the i-th reaction from Group (8) produces the symbols $\spadesuit_j$ for all tape positions different from the new head position $i + d$, encoding that the head is not on those cells after the transition. Furthermore, the following reactions preserve the encoding of the tape cells where the head is *not* located, which are precisely those for which $\spadesuit_j$ has been produced before:

$$(\{\spadesuit_i, a_i\} \cup \heartsuit, \emptyset, \{a_i, \heartsuit^i_\Sigma\}) \qquad \text{for } 1 \le i \le m. \tag{9}$$

Note that the reactions in Groups (7), (8), (9) are the same as in [29, Section 3] with the addition of flag symbols. We now add novel reactions, whose role is to send invalid states to S, whenever multiple alphabetic symbols referring to the same tape cell or multiple state symbols are present simultaneously:

$$(\{a_i, b_i\} \cup \heartsuit, \emptyset, S) \qquad \forall a, b \in \Sigma \quad \text{for } 1 \le i \le m \tag{10}$$

$$(\{q_i, r_j\} \cup \heartsuit, \emptyset, S) \qquad \forall q, r \in Q \quad \text{for } 1 \le i, j \le m. \tag{11}$$

Furthermore, S must be reached whenever a state symbol q_i is present at the same time as the symbol $\spadesuit_i$ because this would indicate that the tape head is not on the cell the state it corresponds to:

$$(\{q_i, \spadesuit_i\} \cup \heartsuit, \emptyset, S) \qquad \forall q \in Q \quad \text{for } 1 \le i \le m \tag{12}$$

Finally, we remark that $\emptyset$ and S are fixed points; moreover, if T is valid then $\mathrm{res}_\mathcal{M}(T)$ is also valid and encodes the next configuration of M. Let us now study the dynamics of invalid states and start with the following useful remark.

Remark 13. The set of reactants of all reactions fully contains the set $\heartsuit$; this ensures that $\mathrm{res}_\mathcal{M}(T) = \emptyset$ for any state T such that

$$T \cap \heartsuit_\Sigma \subsetneq \heartsuit_\Sigma \quad \vee \quad \diamondsuit_Q \notin T.$$

Lemma 14. *If $T \subseteq S$ is an invalid state, then T reaches either $\emptyset$ or S.*

Proof. Let $T \subsetneq S$ be a general state such that $\heartsuit \subseteq T$, otherwise by Remark 13 we have the thesis. We denote

$$T_\Sigma := S_\Sigma \cap T, \quad T_Q := S_Q \cap T, \quad T_\spadesuit := \spadesuit \cap T,$$

thus we can write $T = \heartsuit \cup T_\Sigma \cup T_Q \cup T_\spadesuit$.

If T is valid, by Equation (6) it must be $T_Q = \{q_k\}$ for some $q \in Q$ and $1 \le k \le m$, thus $|T_Q| = 1$. Whenever $|T_Q| > 1$, then a reaction of type (11) is enabled, therefore it would be $\mathrm{res}_\mathcal{M}(T) = S$; and whenever $T_Q = \emptyset$ then no reaction of type (7) is enabled, thus either (i) $\mathrm{res}_\mathcal{M}(T) = S$ if some reactions from Group (10) are enabled or (ii) $\diamondsuit_Q \notin \mathrm{res}_\mathcal{M}(T)$, implying by Remark 13 that $\mathrm{res}^2_\mathcal{M}(T) = \emptyset$. Thus, in the rest of the proof we only consider invalid states such that $T_Q = \{q_k\}$. In the case where $\spadesuit_k \in T_\spadesuit$, then the k-th reaction from Group (12) is enabled, implying $\mathrm{res}_\mathcal{M}(T) = S$; and if $T_\spadesuit \subsetneq \spadesuit \setminus \{\spadesuit_k\}$, then there exists $\spadesuit_l \in \spadesuit \setminus (T_\spadesuit \cup \{\spadesuit_k\})$, thus the l-th reaction of Group (9) is not enabled and $\heartsuit^l_\Sigma \notin \mathrm{res}_\mathcal{M}(T)$ (if no reactions of Group (10) are enabled, otherwise $\mathrm{res}_\mathcal{M}(T) = S$), implying by Remark 13 that $\mathrm{res}^2_\mathcal{M}(T) = \emptyset$. Thus, we restrict the rest of the proof to invalid states such that $T_Q = \{q_k\}$ and $T_\spadesuit = \spadesuit \setminus \{\spadesuit_k\}$. Let us focus on T_Σ. We divide two cases in which T would not be valid.

1. if there exists i such that $a_i, b_i \in T_\Sigma$ for some $a, b \in \Sigma$, the i-th reaction in (10) is enabled, thus $\mathrm{res}_\mathcal{M}(T) = S$;
2. if there exists i such that $a_i \notin T_\Sigma$ for all $a \in \Sigma$, then:
   2a. if $i = k$, no reaction of type (7) is enabled, thus $\heartsuit^k_\Sigma \notin \mathrm{res}_\mathcal{M}(T)$;
   2b. if $i \ne k$, no reaction of type (9) is enabled, thus $\heartsuit^i_\Sigma \notin \mathrm{res}_\mathcal{M}(T)$;
   therefore in both cases $\mathrm{res}^2_\mathcal{M}(T) = \emptyset$.

The only remaining case is when for all $1 \leq i \leq m$ there exists a unique $a \in \Sigma$ such that $a_i \in T_\Sigma$; but since we restricted to the case where $T_Q = \{q_k\}$ and $T_\spadesuit = \spadesuit \setminus \{\spadesuit_k\}$, this implies that T is a valid state. We have proved that if T is not a valid state the orbit starting from T reaches $\varnothing$ or S. $\square$

We are ready to prove Theorem 15 and Lemma 16, which are analogous to Lemma 1 and Theorem 1 from [33] for inhibitorless RS.

Theorem 15. *Let M be a single-tape Turing machine with input a string x over Σ and a unary*[1] *integer $m \geq |x|$. Then, there exist an inhibitorless reaction system $\mathcal{M} = (S, A) \in \mathcal{RS}(\infty, 0)$ and a state $X \subseteq S$ such that M reaches its final state $q^{(f)}$ in t steps on input x using at most m tape cells if and only if $\text{res}^t_{\mathcal{M}}(X) = S$.*

Proof. We modify the construction of the proof of Lemma 14 so as to be able to detect when M exceeds m tape cells. To this aim, we augment S_Q with $\{q_0, q_{m+1} : q \in Q\}$. In this way, whenever one of these elements is generated by a reaction from Group (7) (thus the head of the machine exceeded the array of m cells it is using for the computation), at the next step in $\mathcal{M}$ no reaction from Group (7) is enabled. This implies that $\diamondsuit_Q$ is not generated and by Remark 13 we reach $\varnothing$. We also add a further group of reactions to ensure that if the computation on the Turing machine stops in the final state $q^{(f)}$, in the RS we reach S:

$$(q_i^{(f)}, \varnothing, S) \qquad \text{for } 1 \leq i \leq m. \tag{13}$$

Let T_I be the valid state that encodes the initial configuration of M with input x. Taking $X = T_I$ we have the thesis. $\square$

The following lemma will be crucial to prove the next results. Fixed $k \geq 1$ an integer, it shows how to construct an inhibitorless RS with a cycle of length $\Omega(2^k)$ using only a polynomial (in k) number of reactions and entities.

Lemma 16. *Given any integer $k \geq 1$, there exists an inhibitorless reaction system $C_k = (S_k, A_k) \in \mathcal{RS}(\infty, 0)$ with $|S_k| = \mathcal{O}(k)$ such that any state either reaches a cycle of length $\Omega(2^k)$ or is attracted by $\varnothing$ and S.*

Proof. Let $C = (\{w, r\}, \{0, 1, \rhd\}, \delta)$ be the deterministic Turing machine given by the following transition function:

$$\delta(w, 1) = (w, 0, \rightarrow) \tag{14}$$

$$\delta(w, 0) = (r, 1, \leftarrow) \tag{15}$$

$$\delta(w, \rhd) = (r, \rhd, -) \tag{16}$$

$$\delta(r, 1) = (r, 1, \leftarrow) \tag{17}$$

$$\delta(r, 0) = (r, 0, \leftarrow) \tag{18}$$

$$\delta(r, \rhd) = (w, \rhd, \rightarrow). \tag{19}$$

We defined the transition function as $\delta : Q \times \Sigma \to Q \times \Sigma \times \{\leftarrow, -, \rightarrow\}$, with the clear identification of the set $\{\leftarrow, -, \rightarrow\}$ with the set $\{-1, 0, +1\}$.

The machine C implements a counter that, for any given input integer k, increments a binary number with k digits one by one, starting from 0 and stopping when it exceeds $2^k - 1$. The binary number is stored in the k cells to the right of the symbol $\rhd$ in reverse order, that is, the least significant digit is on the right. For instance, the string $\rhd$10100 represents the number 5; $\rhd$01100 the number 6. In this process, when C reaches the configuration with k ones on the tape (i.e. the counter hits $2^k - 1$), it writes 0 in the k cells after $\rhd$ and stops when it reads a white space in the $(k+1)$-th cell.[2]

Given C and a fixed integer k, we construct an inhibitorless RS $C_k \in \mathcal{RS}(\infty, 0)$ that simulates C over k tape cells to the right of the symbol $\rhd$. We define S_k as

$$S_k := S_\Sigma \cup \heartsuit \cup S_Q \cup \{\spadesuit_j : 0 \leq j \leq k\} \cup \{\blacktriangleleft\}$$

where $S_\Sigma := \{0_j, 1_j : 1 \leq j \leq k\} \cup \{\rhd_0\}$, $S_Q := \{w_j, r_j : 0 \leq j \leq k\}$, $\heartsuit_\Sigma := \{\heartsuit^j_\Sigma : 0 \leq j \leq k\}$, and $\heartsuit := \heartsuit_\Sigma \cup \{\diamondsuit_Q\}$. Thus $|S_k| = 6k + 7 = \mathcal{O}(k)$. The initial configuration of C is represented by the following state in C_k:

$$T_I = \{\rhd_0, 0_1, \ldots, 0_k\} \cup \heartsuit_\Sigma \cup \{r_0, \diamondsuit_Q\} \cup \{\spadesuit_i : 1 \leq i \leq k\}.$$

To define the reactions of C_k, consider the groups of reactions constructed at the beginning of Section 4. To encode Rules (15), (17), (18), we add to C_k the corresponding Groups of reactions (7), (8). Furthermore, since we want to force the symbol $\rhd$ to be always at the first cell of the tape, to encode Rules (16) and (19) we use the following reactions:

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[1] That is, an integer represented in base 1 rather than in base 2, thus encoded by m 1-bits instead of $\log_2 m$ 0/1 bits.

[2] To visualize a similar counter, in which the binary number is stored to the left of some flag symbol without being reversed, visit https://ideonexus.github.io/Explorable-Explanations/math/binarycountingmachine/.

$$(\{w_0, \triangleright_0\} \cup \heartsuit, \varnothing, \{r_0, \triangleright_0, \heartsuit_\Sigma^0, \diamondsuit_Q\})$$

$$(\{w_0, \triangleright_0\} \cup \heartsuit, \varnothing, \{\spadesuit_j : 1 \le j \le m\})$$

$$(\{r_0, \triangleright_0\} \cup \heartsuit, \varnothing, \{w_1, \triangleright_0, \heartsuit_\Sigma^0, \diamondsuit_Q\})$$

$$(\{r_0, \triangleright_0\} \cup \heartsuit, \varnothing, \{\spadesuit_0, \spadesuit_j : 2 \le j \le m\}).$$

We must also control the dynamics of C_k whenever C overflows: we thus need to construct a reaction specific to when we are at position $i = k$ with input symbol 1 and state w, i.e. exactly one step before overflowing. Hence to encode Rule (14) we construct the following reactions:

$$(\{w_i, 1_i\} \cup \heartsuit, \varnothing, \{w_{i+1}, 0_i, \heartsuit_\Sigma^i, \diamondsuit_Q\}) \qquad \text{for } 1 \le i < k \tag{20}$$

$$(\{w_i, 1_i\} \cup \heartsuit, \varnothing, \{\spadesuit_j : 1 \le j \le k, j \ne i+1\}) \qquad \text{for } 1 \le i < k \tag{21}$$

$$(\{w_k, 1_k\} \cup \heartsuit, \varnothing, \{\blacktriangleleft, 0_k, \heartsuit_\Sigma^k\} \cup \spadesuit) \tag{22}$$

$$(\{\blacktriangleleft\} \cup \heartsuit_\Sigma, \varnothing, T_I). \tag{23}$$

We also add the group of reactions (9) to preserve the tape. Recall that if T is a valid state then $\mathrm{res}_{C_k}(T)$ encodes the next configuration of C. Because the reaction (22) generates the symbol $\blacktriangleleft$ instead of $\diamondsuit_Q$ and the reaction (23) produces the initial configuration T_I, the states $\{\mathrm{res}_{C_k}^m(T_I) : m \in \mathbb{N}\}$ form a cycle. The length of the cycle is $\Omega(2^k)$ because for each binary number $x_1 \cdots x_k$ from 0 to $2^k - 1$ we reach a configuration of the type

$$\{\triangleright_0, (x_1)_1, \dots, (x_k)_k\} \cup \heartsuit_\Sigma \cup \{r_0, \diamondsuit_Q\} \cup \{\spadesuit_i : 1 \le i \le k\}. \tag{24}$$

Remark that the way we defined the reactions guarantees that a valid state always contains $\triangleright_0$.

Claim 1. *Any valid state T always reaches the cycle starting from T_I.*

Proof. If T encodes a configuration with state w, the computation either overflows or reaches a configuration with state r; whenever the state is r, the computation always goes back to $\triangleright$ preserving the tape, thus reaches a configuration of the type (24). ■

Finally, to control invalid states, we add the following reactions (which are never enabled by valid states) that are analogous to the reactions (10), (11), (12):

$$(\{a_i, b_i\} \cup \heartsuit, \varnothing, S_k) \qquad \forall a, b \in \{0, 1, \triangleright\} \quad \text{for } 0 \le i \le k \tag{25}$$

$$(\{q_i, q'_j\} \cup \heartsuit, \varnothing, S_k) \qquad \forall q, q' \in \{w, r\} \quad \text{for } 0 \le i, j \le k \tag{26}$$

$$(\{q_i, \spadesuit_i\} \cup \heartsuit, \varnothing, S_k) \qquad \forall q \in \{w, r\} \quad \text{for } 0 \le i \le k \tag{27}$$

$$(\{q_i, \blacktriangleleft\} \cup \heartsuit, \varnothing, S_k) \qquad \forall q \in \{w, r\} \quad \text{for } 0 \le i \le k \tag{28}$$

where in Group (28) we treat $\blacktriangleleft$ as a state of C.

Claim 2. *Any invalid state reaches either $\varnothing$, S_k or T_I.*

Proof. Let $T \subseteq S_k$ be any invalid state of C_k. If $T \cap \heartsuit_\Sigma \subsetneq \heartsuit_\Sigma$ then no reaction is enabled, so we get $\mathrm{res}_{C_k}(T) = \varnothing$. Analogously to the proof of Lemma 14, we study what happens for $T = \heartsuit_\Sigma \cup T_\Sigma \cup T_Q \cup T_\spadesuit \cup T_{\diamondsuit_Q}$, where $T_{\diamondsuit_Q} = T \cap \{\diamondsuit_Q\}$ and $T_Q = T \cap (Q \cup \{\blacktriangleleft\})$. Consider the case where $T_{\diamondsuit_Q} = \varnothing$. In this case, no reaction can be enabled, except for (23): if T enables (23) we have $\mathrm{res}_{C_k}(T) = T_I$, otherwise $\mathrm{res}_{C_k}(T) = \varnothing$. Now consider the case where $T_{\diamondsuit_Q} = \{\diamondsuit_Q\}$, therefore $T = \heartsuit \cup T_\Sigma \cup T_Q \cup T_\spadesuit$. If $|T_Q| > 1$ then $\mathrm{res}_{C_k}(T) = S_k$, thus we divide into three cases:

- If $T_Q = \varnothing$, if a reaction of Group (25) is enabled then $\mathrm{res}_{C_k}(T) = S_k$, otherwise $(S_Q \cup \spadesuit) \cap \mathrm{res}_{C_k}(T) = \varnothing$, since no reactions from Groups (7), (8) are enabled. Therefore, $\mathrm{res}_{C_k}(T)$ could only enable reactions of Group (25); we conclude that either $\mathrm{res}_{C_k}^2(T) = \varnothing$ or $\mathrm{res}_{C_k}(T) = S_k$.
- If $T_Q = \{q_k\}$ for some k, then we proceed similarly to the proof of Lemma 14.
- If $T_Q = \{\blacktriangleleft\}$, then $\mathrm{res}_{C_k}(T) = T_I \cup \mathrm{res}_{C_k}(\heartsuit \cup T_\Sigma \cup T_\spadesuit)$. If a reaction from Group (25) is enabled by $\heartsuit \cup T_\Sigma \cup T_\spadesuit$ then $\mathrm{res}_{C_k}(T) = S_k$. So suppose that none of them is enabled, then only reactions from Group (9) are enabled, thus $\mathrm{res}_{C_k}(\heartsuit \cup T_\Sigma \cup T_\spadesuit) \subseteq \heartsuit_\Sigma \cup S_\Sigma$. If $\mathrm{res}_{C_k}(\heartsuit \cup T_\Sigma \cup T_\spadesuit) \cap S_\Sigma \not\subseteq T_I$, then at the next step one reaction of Group (25) is enabled. We conclude that in this case we either reach T_I or S_k. ■

The thesis follows. □

We are now ready to prove the hardness of the problems in Table 1. From Lemma 8, we know that for $\mathcal{A} \in \mathcal{RS}(\infty, 0)$ a global attractor given by two fixed points must be of the form $\mathcal{U} = \{\mathrm{res}^n_{\mathcal{A}}(\varnothing), \mathrm{res}^m_{\mathcal{A}}(S)\}$ for some integer $n, m \geq 0$; we prove that determining if one such $\mathcal{U}$ is a global attractor is **PSPACE**-complete. We start by proving in Theorem 17 that already determining whether the special case $\mathcal{U} = \{\varnothing, S\}$ is a global attractor is **PSPACE**-complete.

Theorem 17. *Given $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ such that $\varnothing$ and S are fixed points, it is* **PSPACE***-complete to decide if $\{\varnothing, S\}$ is a global attractor.*

Proof. We prove the hardness of the problem by a reduction from the following **PSPACE**-complete problem: given a deterministic Turing machine M, a string x and a unary integer m, does M accept x without using more than m tape cells? Let $M = (Q, \Sigma, \delta)$ be a single-tape deterministic Turing machine with input x and a unary integer $m \geq |x|$. We construct a RS $\mathcal{M} = (S_{\mathcal{M}}, A_{\mathcal{M}}) \in \mathcal{RS}(\infty, 0)$ using Theorem 15. Let k be an integer such that $m \cdot |Q| \cdot |\Sigma|^m \leq 2^k$ and construct a RS $\mathcal{C} = \mathcal{C}_k = (S_{\mathcal{C}}, A_{\mathcal{C}}) \in \mathcal{RS}(\infty, 0)$ as in Lemma 16. Let $S_{\mathcal{M}}$ be the background set of $\mathcal{M}$ and $S_{\mathcal{C}}$ be the background set of $\mathcal{C}$, such that $S_{\mathcal{M}} \cap S_{\mathcal{C}} = \varnothing$. The entities in $S_{\mathcal{M}}$ (resp. $S_{\mathcal{C}}$) and the states over $\mathcal{M}$ (resp. $\mathcal{C}$) will be denoted with $T^{\mathcal{M}}$ (resp. $T^{\mathcal{C}}$). Let $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ such that $S = S_{\mathcal{C}} \cup S_{\mathcal{M}}$ and $A = A'_{\mathcal{C}} \cup A'_{\mathcal{M}}$ where $A'_{\mathcal{C}}$ is the set of reactions $A_{\mathcal{C}}$ from Lemma 16 (replacing S_k by S in reactions (25), (26), (28)) and $A'_{\mathcal{M}}$ is the set of reactions $A_{\mathcal{M}}$ from Theorem 15 modified as follows: the entity $\diamond^{\mathcal{C}}_{Q} \in S_{\mathcal{C}}$ is added to the reactants of all reactions and $S_{\mathcal{M}}$ is replaced by S in reactions (10), (11), (12), (13). Furthermore, we replace the reaction (23) of $A'_{\mathcal{C}}$ with the following reaction

$$(\{\blacktriangleleft^{\mathcal{C}}\} \cup \heartsuit^{\mathcal{C}}_{\Sigma}, \varnothing, T^{\mathcal{C}}_{I} \cup T^{\mathcal{M}}_{I}) \tag{29}$$

where the state $T^{\mathcal{M}}_{I}$ represents the initial configuration of M. In this way, whenever the counter overflows, implying that $\diamond^{\mathcal{C}}_{Q}$ does not appear and $\blacktriangleleft^{\mathcal{C}}$ is generated, none of the reactions of $\mathcal{M}$ is enabled, thus reaction (29) resets $\mathcal{C}$ and $\mathcal{M}$ to the initial state.

We now study the dynamics of $\mathcal{A}$. We will denote by $\mathrm{res}_{\mathcal{C}}(T)$ (resp. $\mathrm{res}_{\mathcal{M}}(T)$) the result function of $\mathcal{A}$ restricted to $A'_{\mathcal{C}}$ (resp. to $A'_{\mathcal{M}}$). Let $T = T^{\mathcal{C}} \cup T^{\mathcal{M}} \subseteq S$ given by the union of two valid states of $\mathcal{C}$ and $\mathcal{M}$. Since the background sets of the two reaction systems are disjunct, we have that $\mathrm{res}_{\mathcal{A}}(T^{\mathcal{C}} \cup T^{\mathcal{M}}) = \mathrm{res}_{\mathcal{C}}(T^{\mathcal{C}}) \cup \mathrm{res}_{\mathcal{M}}(T^{\mathcal{M}})$. Recall that by Claim 1, there exists $t \in \mathbb{N}$ such that $\mathrm{res}^t_{\mathcal{C}}(T^{\mathcal{C}}) = T^{\mathcal{C}}_{I}$. If the computation of M starting from the configuration $T^{\mathcal{M}}$ halts, then we reach the state S; otherwise, if M does not halt or uses more than m tape cells (thus $T^{\mathcal{M}}$ reaches $\varnothing$), the counter overflows and both M and $\mathcal{C}$ are reset to the initial state $T^{\mathcal{C}}_{I} \cup T^{\mathcal{M}}_{I}$. Finally, since the counter resets after that all possible configurations over m cells of M have been possibly reached, we have that $T^{\mathcal{C}}_{I} \cup T^{\mathcal{M}}_{I}$ is part of a cycle if and only if M does not halt or uses more than m cells; furthermore, $T^{\mathcal{C}}_{I} \cup T^{\mathcal{M}}_{I}$ reaches S if and only if M halts with input x using at most m tape cells. If we can prove that, whenever we have an invalid configuration of $\mathcal{C}$ or $\mathcal{M}$, the state reaches $\varnothing$, S or $T^{\mathcal{C}}_{I} \cup T^{\mathcal{M}}_{I}$, we obtain the thesis.

Now suppose that $T^{\mathcal{M}}$ is an invalid state for $\mathcal{M}$, then $T^{\mathcal{M}}$ either reaches $\varnothing$ or S. In the former case, the dynamics is completely controlled by $T^{\mathcal{C}}$, thus either we reach $\varnothing$ or S, or we enter in the loop of $T^{\mathcal{C}}_{I}$, thus everything is reset to $T^{\mathcal{C}}_{I} \cup T^{\mathcal{M}}_{I}$. We must study the case where $T^{\mathcal{M}}$ is a valid state but $T^{\mathcal{C}}$ is invalid. In this case, if $T^{\mathcal{C}}$ reaches S then $T^{\mathcal{C}} \cup T^{\mathcal{M}}$ reaches S; if $T^{\mathcal{C}}$ reaches $T^{\mathcal{C}}_{I}$ then either $T^{\mathcal{M}}$ carries on the computation until the counter overflows or $T^{\mathcal{M}}$ reaches the final state; if $T^{\mathcal{C}}$ reaches $\varnothing$, then $\diamond^{\mathcal{C}}_{Q}$ is no longer present, implying that the computation of $T^{\mathcal{M}}$ stops and $T^{\mathcal{M}} \cup T^{\mathcal{C}}$ reaches $\varnothing$.

We conclude that M accepts x using less than m tape cells if and only if $\{\varnothing, S\}$ is a global attractor for $\mathcal{A}$. Since the map $(M, x, 1^m) \mapsto \mathcal{A}$ is computable in polynomial time by the constructions of Lemma 16 and Theorem 15, we have that deciding if $\{\varnothing, S\}$ is a global attractor for an inhibitorless reaction system is **PSPACE**-hard. ☐

The following two corollaries can be derived from Theorem 17.

Corollary 18. *Let $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ and $\varnothing \subsetneq T_1 \subsetneq T_2 \subsetneq S$ be fixed points such that $T_1 = \mathrm{res}^n_{\mathcal{A}}(\varnothing)$ and $T_2 = \mathrm{res}^m_{\mathcal{A}}(S)$ for some integer $n, m \geq 0$. It is* **PSPACE***-complete to decide if $\{T_1, T_2\}$ is a global attractor.*

Proof. Given $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ such that $\varnothing$ and S are fixed points, we can construct $\mathcal{B} = (S', B) \in \mathcal{RS}(\infty, 0)$ as done in Corollary 11. It follows that $\{\varnothing, S\}$ is a global attractor for $\mathcal{A}$ if and only if $\{\mathrm{res}_{\mathcal{B}}(\varnothing), \mathrm{res}_{\mathcal{B}}(S')\}$ is a global attractor for $\mathcal{B}$. ☐

Corollary 19. *Given $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$, deciding if there exists a global attractor given by two fixed points is* **PSPACE***-complete.*

Proof. Let $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ such that $\varnothing$ and S are fixed points. If $\mathcal{A}$ has a global attractor given by two fixed points, it must be $\{\varnothing, S\}$, as if we have a global attractor, all the fixed points and cycles must belong to it; see Observation 2. Therefore, $\mathcal{A}$ has a global attractor given by two fixed points if and only if $\{\varnothing, S\}$ is a global attractor. Since the former problem is **PSPACE**-complete by Theorem 17, we have the thesis. ☐

We now move on to prove that the problems of deciding whether (i) a given state is part of a cycle, (ii) two reaction systems have the same set of cycles, and (iii) two reaction systems have at least one cycle in common are all **PSPACE**-complete when restricted to inhibitorless reaction systems. These results, respectively stated in Theorems 20, 21 and 22, are all almost straightforward implications of Theorem 17.

Theorem 20. *Given $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ and a state $T \subseteq S$, it is* **PSPACE***-complete to decide whether T is part of a cycle.*

Proof. We reduce from the same **PSPACE**-complete problem we used in the proof of Theorem 17: given a deterministic Turing machine M, a string x and a unary integer m, does M accept x without using more than m tape cells? By constructing in polynomial time a reaction system $\mathcal{A}$ as in the proof of Theorem 17 and choosing $T = T_I^{\mathcal{C}} \cup T_I^{\mathcal{M}}$, we find that T belongs to a cycle if and only if M does not halt or uses more than m cells. $\square$

Theorem 21. *Given $\mathcal{A}, \mathcal{B} \in \mathcal{RS}(\infty, 0)$ over the same background set S, it is* **PSPACE***-complete to decide whether they share all their cycles.*

Proof. We reduce again from the **PSPACE**-complete problem of deciding, given a deterministic Turing machine M, a string x and a unary integer m, if M accepts x without using more than m tape cells. Following the reduction of Theorem 17, we construct the map $(M, x, 1^m) \mapsto (\mathcal{A}, \mathcal{B})$, where $\mathcal{B}$ has $(S, \varnothing, S)$ as its only reaction. In this way $\mathcal{A}$ and $\mathcal{B}$ share all cycles if and only if the only fixed points of $\mathcal{A}$ are $\varnothing$ and S, and this happens if and only if M accepts x using at most m tape cells. $\square$

Theorem 22. *Given $\mathcal{A}, \mathcal{B} \in \mathcal{RS}(\infty, 0)$ over the same background set S, it is* **PSPACE***-complete to decide whether they share a common cycle.*

Proof. Once again, we reduce from the **PSPACE**-complete problem of deciding, given a deterministic Turing machine M, a string x and a unary integer m, if M accepts x without using more than m tape cells. Let $M = (Q, \Sigma, \delta)$ be a single-tape deterministic Turing machine with input x and a unary integer $m \geq |x|$. We construct a RS $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ as in Theorem 17. We add to the background set of $\mathcal{A}$ a new symbol $\clubsuit \notin S$. Let $\mathcal{B} = (S \cup \{\clubsuit\}, B) \in \mathcal{RS}(\infty, 0)$, where $B = A \cup \{(S, \varnothing, S \cup \{\clubsuit\}), (\varnothing, \varnothing, \heartsuit_\Sigma^{\mathcal{C}} \cup \heartsuit_\Sigma^{\mathcal{M}})\}$. In this way, $\varnothing$ and S are fixed points of $\mathcal{A}$ but not of $\mathcal{B}$. Recall that $\mathcal{A}$ has a cycle given by valid states different from $\varnothing$ and S if and only if M halts for x within m tape cells. Since $\mathcal{A}$ and $\mathcal{B}$ coincide on valid states, we deduce that $\mathcal{A}$ and $\mathcal{B}$ share a common cycle if and only if M with input x halts within m tape cells. $\square$

5. Global attractors of reactantless reaction systems

5.1. *Existence of a global fixed-point attractor*

We begin this section by characterizing global fixed-point attractors when the function is antitone. Corollary 24, analogously to Corollary 4 for the monotone case, will then provide a criterion to decide the existence of a global fixed-point attractor for antitone functions in polynomial time.

Proposition 23. *Let S be a finite set, $f : 2^S \to 2^S$ antitone and T a fixed point for f. Then, T is a global fixed-point attractor for f if and only if T is a global fixed-point attractor for f^2.*

Proof. $\boxed{\Rightarrow}$ Since T is a fixed point for f, it is also a fixed point for f^2. We need to prove that T is a global attractor for f^2, but since for every state $T' \subseteq S$ there exists $t \in \mathbb{N}$ such that $f^t(T') = T$, then $(f^2)^t(T') = f^{2t}(T') = f^2(T) = T$.

$\boxed{\Leftarrow}$ Consider T a global fixed-point attractor for f^2. Then it must hold that $f(T) = T$, as otherwise, $f(T) \neq T$ would imply that $f^2(f(T)) = f(T)$ and thus $f(T)$ would be a fixed point for f^2 different from T, which is a contradiction by Observation 2. $f(T) = T$ implies that T is also a global fixed-point attractor for f, because for every $T' \subseteq S$, T' reaches T in t steps through f^2, thus T' reaches T in $2t$ steps through f. $\square$

Corollary 24. *Given S a finite set and $f : 2^S \to 2^S$ antitone, a global fixed-point attractor for f exists if and only if there exists a global fixed-point attractor for f^2.*

Proposition 23 and Corollary 24 can be applied straightforwardly to result functions of reactantless reaction systems, leading to the following two results.

Corollary 25. *Given a RS $\mathcal{A} = (S, A) \in \mathcal{RS}(0, \infty)$ and a state $T \subseteq S$, deciding if T is a global fixed-point attractor of $\mathcal{A}$ is in* **P**.

Proof. Since $\text{res}_{\mathcal{A}}$ is antitone [27], Proposition 23 applies. Therefore, T is a global attractor for $\mathcal{A}$ if and only if T is a global fixed-point attractor for $\text{res}^2_{\mathcal{A}}$. Since $\text{res}^2_{\mathcal{A}}$ is monotone, we can proceed as in the proof of Corollary 5, and decide whether T is a global attractor simply by evaluating $\text{res}_{\mathcal{A}}$ at most $2|S|$ times. $\square$

Corollary 26. *Given a RS $\mathcal{A} = (S, A) \in \mathcal{RS}(0, \infty)$, deciding whether there exists a global fixed-point attractor of $\mathcal{A}$ is in* **P**.

Proof. Since $\text{res}_{\mathcal{A}}$ is antitone [27], Corollary 24 applies, which implies that there exists a global fixed-point attractor for $\text{res}_{\mathcal{A}}$ if and only if there exists a global fixed-point attractor for $\text{res}^2_{\mathcal{A}}$. We conclude as in Corollary 25. $\square$

(a) A global 2-cycle attractor.

(b) A global attractor consisting of two fixed points.

Fig. 3. Representation of the dynamics of Example 28.

5.2. *Existence of a global cycle attractor*

We begin this section by showing, in Proposition 27, that a global k-cycle attractor cannot exist for any antitone function for any $k > 2$: see also Example 28.

Proposition 27. *Let $\mathcal{U}$ be a global cycle attractor for an antitone function $f : 2^S \to 2^S$, then there exists $T \subseteq S$ such that either $\mathcal{U} = \{T\}$ or $\mathcal{U} = \{T, f(T)\}$.*

Proof. Let $f^2(\mathcal{U}) := \{f^2(U) : U \in \mathcal{U}\}$; this is a global attractor invariant set for f^2. Suppose $\mathcal{U}$ is a $(2k+1)$-cycle for some $k \geq 0$: then $f^2(\mathcal{U})$ is also a $(2k+1)$-cycle. Since by Lemma 7 every global attractor invariant set for a monotone function must contain a fixed point, and since f being antitone implies f^2 being monotone, it must be $k = 0$, and thus $\mathcal{U} = f^2(\mathcal{U}) = \{T\}$ must be a global fixed-point attractor for f^2. Suppose now $\mathcal{U}$ is a $(2k)$-cycle for some $k \geq 1$: then $f^2(\mathcal{U})$ consists of two k-cycles. Since one of the two cycles must be a fixed point by Lemma 7, it must be $k = 1$ and thus $\mathcal{U} = \{T, f(T)\}$ for some $T \subseteq S$. ☐

Example 28. Let $S = \{a, b\}$ and $f : 2^S \to 2^S$ given by:

$$f(\varnothing) = \{a, b\}; \quad f(\{a\}) = \varnothing; \quad f(\{b\}) = \{a\}; \quad f(\{a, b\}) = \varnothing.$$

f is clearly antitone and in the dynamics, we have a global 2-cycle attractor $\{\varnothing, S\}$: see Fig. 3a. Consider now $f^2 : 2^S \to 2^S$, given by

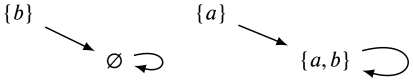
$$f^2(\varnothing) = \varnothing; \quad f^2(\{a\}) = \{a, b\}; \quad f^2(\{b\}) = \varnothing; \quad f^2(\{a, b\}) = \{a, b\}.$$

f^2 has a global attractor consisting of two fixed points; see Fig. 3b. ⌟

From the proof of Proposition 27, we deduce that an antitone function $f : 2^S \to 2^S$ has a global 2-cycle attractor if and only if $f^2 : 2^S \to 2^S$ has a global attractor consisting of two fixed points.

The rest of this section is devoted to proving that deciding whether a reactantless RS has a global 2-cycle attractor reduces to the problem of Theorem 17 for inhibitorless systems, and it is, therefore, **PSPACE**-complete as well. We begin with an example illustrating the workings of the reduction we later provide in Theorem 30.

Example 29. Let $S = \{a, b\}$ and $\mathcal{A} = (S, A)$ an inhibitorless reaction system where $A = \{(\{a\}, \varnothing, \{a, b\})\}$. As already seen in Example 28, in the dynamics of $\mathcal{A}$ there are two fixed points that form together a global attractor (same dynamics as Fig. 3b):



We want to construct a reactantless reaction system that can reproduce the dynamics of $\mathcal{A}$ for states $\varnothing \subsetneq T \subsetneq S$ and transform the global attractor of $\mathcal{A}$, consisting of two fixed points, into a global 2-cycle attractor. We thus construct $\mathcal{B} = (S', B)$ where $S' = \{a, b, \heartsuit, \spadesuit\}$ and B is given by the following reactions:

$$(\varnothing, \{a, \heartsuit\}, \{a, \heartsuit\})$$
$$(\varnothing, \{b, \heartsuit\}, \{b, \heartsuit\})$$
$$(\varnothing, \{a, \spadesuit\}, \{a, b, \spadesuit\})$$
$$(\varnothing, \{a, b, \heartsuit\}, \{a, b, \heartsuit, \spadesuit\})$$
$$(\varnothing, \{a, b, \spadesuit\}, \{a, b, \heartsuit, \spadesuit\})$$
$$(\varnothing, \{\heartsuit, \spadesuit\}, \{a, b, \heartsuit, \spadesuit\}).$$

It is straightforward to verify that $\mathrm{res}_{\mathcal{B}}(\{b, \spadesuit\}) = \{a, \heartsuit\}$ and $\mathrm{res}_{\mathcal{B}}(\{a, \spadesuit\}) = \{b, \heartsuit\}$, thus

$$\mathrm{res}^2_{\mathcal{B}}(\{b, \spadesuit\}) = \varnothing \quad \text{and} \quad \mathrm{res}^2_{\mathcal{B}}(\{a, \spadesuit\}) = \{a, b, \spadesuit\}.$$

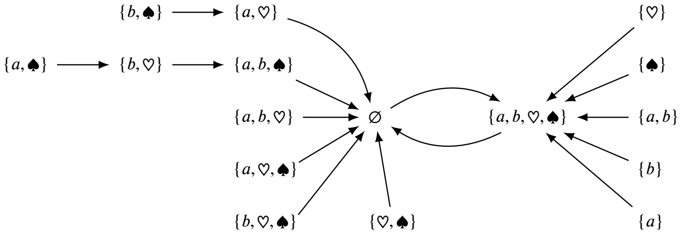


Fig. 4. Dynamics of the RS $\mathcal{B}$ in Example 29.

Note that in the original inhibitorless RS $\mathcal{A}$ we have $\text{res}_{\mathcal{A}}(\{b\}) = \emptyset$ and $\text{res}_{\mathcal{A}}(\{a\}) = \{a, b\}$, thus $\mathcal{B}$ can reproduce the dynamics of $\mathcal{A}$ in two steps starting from the states $\{a, ♠\}$ and $\{b, ♠\}$ and going through the states $\{a, ♡\}$ and $\{b, ♡\}$. The last three reactions of B ensure that there is a global 2-cycle attractor, as all the states except for $\{a, ♠\}$, $\{b, ♠\}$, and $\{b, ♡\}$ reach the 2-cycle $\{\emptyset, S'\}$ in one step, which makes it a global 2-cycle attractor. The dynamics of $\mathcal{B}$ is represented in Fig. 4. ⌟

In Theorem 30, we extend and generalize the construction of Example 29 to any $\mathcal{A} \in \mathcal{RS}(\infty, 0)$ to reduce the problem of deciding whether $\mathcal{U} = \{\emptyset, S\}$ is a global attractor in inhibitorless reaction systems to the problem of deciding the existence of a global 2-cycle attractor in reactantless reaction systems.

Theorem 30. *Given $\mathcal{A} = (S, A) \in \mathcal{RS}(0, \infty)$, deciding if there exists a global 2-cycle attractor is* **PSPACE***-complete.*

Proof. Given $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ such that $\emptyset$ and S are fixed points, we want to construct in polynomial time a RS $\mathcal{B} \in \mathcal{RS}(0, \infty)$ such that $\{\emptyset, S\}$ is a global attractor for $\mathcal{A}$ if and only if there exists a global 2-cycle attractor for $\mathcal{B}$. We reduce from the problem of deciding if $\mathcal{U} = \{\emptyset, S\}$ is a global attractor in inhibitorless reaction systems (see Theorem 17). We construct a reactantless RS $\mathcal{B} := (S', B)$, with $S' := S \cup \{♡, ♠\}$ and B is given by the following reactions:

$$(\emptyset, \{s, ♡\}, \{s, ♡\}) \qquad \text{for } s \in S \tag{30}$$

$$(\emptyset, R_a \cup \{♠\}, P_a \cup \{♠\}) \qquad \text{for } a = (R_a, \emptyset, P_a) \in A \tag{31}$$

$$(\emptyset, S \cup \{♡\}, S \cup \{♡, ♠\}) \tag{32}$$

$$(\emptyset, S \cup \{♠\}, S \cup \{♡, ♠\}) \tag{33}$$

$$(\emptyset, \{♡, ♠\}, S \cup \{♡, ♠\}). \tag{34}$$

Claim 3. *All states of $\mathcal{B}$ of the forms $\{♠\}, \{♡\}$, $S \cup \{♡\}$, $S \cup \{♠\}$, T, and $T \cup \{♡, ♠\}$, for all $T \subseteq S$, reach $\{\emptyset, S'\}$ in one step. Furthermore, $\text{res}_{\mathcal{B}}(\emptyset) = S'$ and $\text{res}_{\mathcal{B}}(S') = \emptyset$.*

Proof. We immediately note that for any $T \subseteq S$ we have $\text{res}_{\mathcal{B}}(T) = S \cup \{♡, ♠\} = S'$ since reaction (34) is enabled, and $\text{res}_{\mathcal{B}}(T \cup \{♡, ♠\}) = \emptyset$ since no reaction is enabled. By reactions (32) and (33), we also have $\text{res}_{\mathcal{B}}(\{♠\}) = \text{res}_{\mathcal{B}}(\{♡\}) = S \cup \{♡, ♠\} = S'$. Furthermore, since $\text{res}_{\mathcal{A}}(\emptyset) = \emptyset$, then $R_a \neq \emptyset$ for each $a \in A$, thus $S \cup \{♡\}$ does not enable any reaction of Group (31), thus $\text{res}_{\mathcal{B}}(S \cup \{♡\}) = \emptyset$, as well as $\text{res}_{\mathcal{B}}(S \cup \{♠\}) = \emptyset$. Finally, since all the reactions are enabled by $\emptyset$, and no reaction is enabled by $S' = S \cup \{♡, ♠\}$, we have that $\text{res}_{\mathcal{B}}(\emptyset) = S'$ and $\text{res}_{\mathcal{B}}(S') = \emptyset$. See also Fig. 5 for a visual representation of the dynamics. ■

Claim 4. *The states $\{♠\}$, $\{♡\}$, $\{♡, ♠\}$, S, $S \cup \{♡\}$, T, and $T \cup \{♡, ♠\}$, for all $\emptyset \subsetneq T \subsetneq S$, cannot be reached from any states.*

Proof. From the definition of RS, there are no reactions of the type $(R_a, \emptyset, \emptyset)$, because in any case, they do not affect the dynamics of $\mathcal{A}$. Therefore $\text{en}_{\mathcal{A}}(T) = \emptyset$ if and only if $\text{res}_{\mathcal{A}}(T) = \emptyset$. This implies that Group (31) of the reactions of $\mathcal{B}$ does not contain any reactions of the form $(\emptyset, R_a \cup \{♠\}, \{♠\})$, implying that the state $\{♠\}$ cannot be reached from any state. With a similar reasoning we deduce that also states $\{♡\}$, $\{♡, ♠\}$, S, and T for all $\emptyset \subsetneq T \subsetneq S$ cannot be reached from any state.

Furthermore, none of the states of the form $T \cup \{♡, ♠\}$ with $\emptyset \subsetneq T \subsetneq S$ can be reached from any state: indeed, suppose for a contradiction that $\text{res}_{\mathcal{B}}(T') = T \cup \{♡, ♠\}$ for some $T' \subseteq S'$ and $\emptyset \subsetneq T \subsetneq S$. In order to obtain $♡$ in the product, T' must enable some reactions from Group (30); and to obtain $♠$, it must also enable reactions from Group (31). This implies $♡, ♠ \notin T'$, thus $T' \subseteq S$ and thus, by Claim 3, $\text{res}_{\mathcal{B}}(T') = S \cup \{♡, ♠\}$, which is a contradiction because by hypothesis $T \subsetneq S$. Finally, $S \cup \{♡\}$ cannot be reached from any state U because this would require all and only the reactions from Group (30) to be enabled in U, which can happen only if $U = \{♠\}$; but then reaction (32) is enabled as well, and indeed $\text{res}_{\mathcal{B}}(\{♠\}) = S'$ by Claim 3. ■

It remains to determine the dynamics for the states of the form $T \cup \{♠\}$ and $T \cup \{♡\}$ for some $\emptyset \subsetneq T \subsetneq S$. Because of the reactions from Group (30), we obtain

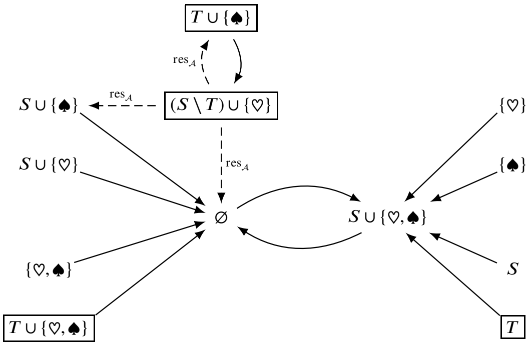


Fig. 5. Dynamics of the RS $\mathcal{B}$ in the reduction of Theorem 30. The states T, $T \cup \{\heartsuit, \spadesuit\}$, $T \cup \{\spadesuit\}$ and $(S \setminus T) \cup \{\heartsuit\}$ are a synthetic representation of the $2^S - 2$ states (one fore each $\varnothing \subsetneq T \subsetneq S$) of each type. The boxes around states $T \cup \{\spadesuit\}$ and $(S \setminus T) \cup \{\heartsuit\}$ hide the more refined dynamics for those states; dashed arcs represent the three existing possibilities for the dynamics of the states belonging to the boxes, as described after Claim 4.

$$\mathrm{res}_{\mathcal{B}}(T \cup \{\spadesuit\}) = (S \setminus T) \cup \{\heartsuit\}; \tag{35}$$

and because of the reactions from Group (31), in turn we have

$$\mathrm{res}_{\mathcal{B}}((S \setminus T) \cup \{\heartsuit\}) = \begin{cases} \mathrm{res}_{\mathcal{A}}(T) \cup \{\spadesuit\} & \text{if } \mathrm{en}_{\mathcal{A}}(T) \neq \varnothing \\ \varnothing & \text{otherwise,} \end{cases} \tag{36}$$

since $(S \setminus T) \cup \{\heartsuit\}$ enables $(\varnothing, R_a \cup \{\spadesuit\}, P_a \cup \{\spadesuit\})$ if and only if $(S \setminus T) \cap R_a = \varnothing$, which is the case if and only if $R_a \subseteq T$ and thus T enables $(R_a, \varnothing, P_a)$ in $\mathcal{A}$. As remarked in Claim 4, we have that $\mathrm{res}_{\mathcal{A}}(T) = \varnothing$ if and only if $\mathrm{en}_{\mathcal{A}}(T) = \varnothing$, which is true if and only if $\mathrm{res}_{\mathcal{B}}((S \setminus T) \cup \{\heartsuit\}) = \varnothing$. We have obtained the following formula:

$$\mathrm{res}^2_{\mathcal{B}}(T \cup \{\spadesuit\}) = \begin{cases} \mathrm{res}_{\mathcal{A}}(T) \cup \{\spadesuit\} & \text{if } \mathrm{en}_{\mathcal{A}}(T) \neq \varnothing \\ \varnothing & \text{otherwise.} \end{cases} \tag{37}$$

Therefore, iterating (37), if $\mathrm{res}^i_{\mathcal{A}}(T) \notin \{\varnothing, S\}$ for all $i = 1, \dots, k-1$ we obtain

$$\mathrm{res}^{2k}_{\mathcal{B}}(T \cup \{\spadesuit\}) = \begin{cases} \mathrm{res}^k_{\mathcal{A}}(T) \cup \{\spadesuit\} & \text{if } \mathrm{res}^k_{\mathcal{A}}(T) \neq \varnothing \\ \varnothing & \text{otherwise.} \end{cases} \tag{38}$$

Note that the states of the form $T \cup \{\heartsuit\}$ with $\varnothing \subsetneq T \subsetneq S$ coincide with the states of the form $(S \setminus T) \cup \{\heartsuit\}$; in particular, any such state $T \cup \{\heartsuit\}$ is reached from $(S \setminus T) \cup \{\spadesuit\}$ by Equation (35), and reaches either $\varnothing$ or $\mathrm{res}_{\mathcal{A}}(S \setminus T) \cup \{\spadesuit\}$ according to Equation (36). In Fig. 5, the states of the form $T \cup \{\heartsuit\}$ and $T \cup \{\spadesuit\}$ are compactly represented as boxed states, and their dynamics are not completely represented for the sake of readability.

We observe that the only candidate global 2-cycle attractor for $\mathcal{B}$ is $\{\varnothing, S'\}$, as it is a 2-cycle by Claim 3 and it is the only candidate global attractor by Claim 4 and the discussion below its proof. The next claim gives us the thesis.

Claim 5. *The state $\{\varnothing, S\}$ is a global attractor for $\mathcal{A}$ if and only if $\{\varnothing, S'\}$ is a global attractor for $\mathcal{B}$.*

Proof.

$\boxed{\Rightarrow}$ Let $\varnothing \subsetneq T \subsetneq S$: in this case, we already proved in Claim 3 that T and $T \cup \{\heartsuit, \spadesuit\}$ reach $\{\varnothing, S'\}$ in one step. We need to prove that $T \cup \{\spadesuit\}$ and $T \cup \{\heartsuit\}$ reach $\{\varnothing, S'\}$. By hypothesis, $\exists k \in \mathbb{N}$ such that $\mathrm{res}^k_{\mathcal{A}}(T) \in \{\varnothing, S\}$. Let k be the minimum number that satisfies this property, implying that $\mathrm{res}^i_{\mathcal{A}}(T) \notin \{\varnothing, S\}$ for $i = 1, \dots, k-1$. Since by hypothesis $\mathrm{res}^k_{\mathcal{A}}(T) \in \{\varnothing, S\}$, there are two cases: if $\mathrm{res}^k_{\mathcal{A}}(T) = S$, then, by Equation (38), $\mathrm{res}^{2k}_{\mathcal{B}}(T \cup \{\spadesuit\}) = S \cup \{\spadesuit\}$, implying that $\mathrm{res}^{2k+1}_{\mathcal{B}}(T \cup \{\spadesuit\}) = \mathrm{res}_{\mathcal{B}}(S \cup \{\spadesuit\}) = \varnothing$ (by Claim 3). Otherwise, $\mathrm{res}^k_{\mathcal{A}}(T) = \varnothing$ and thus $\mathrm{res}^{2k}_{\mathcal{B}}(T \cup \{\spadesuit\}) = \varnothing$ by Equation (38). In any case, $T \cup \{\spadesuit\}$ reaches $\{\varnothing, S'\}$ in at most $2k+1$ steps. For the state $T \cup \{\heartsuit\}$, we can reduce to the previous case using Equation (36). Together with Claim 3, we obtain that if $\{\varnothing, S\}$ is a global attractor for $\mathcal{A}$ then $\{\varnothing, S'\}$ is a global attractor for $\mathcal{B}$.

$\boxed{\Leftarrow}$ Let $\varnothing \subsetneq T \subsetneq S$: by hypothesis, there exists $k \in \mathbb{N}$ such that $\mathrm{res}^k_{\mathcal{B}}(T \cup \{\spadesuit\}) \in \{\varnothing, S'\}$. Let k be the minimum number that satisfies that property. We want to prove that T is always attracted by $\{\varnothing, S\}$. We define two cases, depending on whether k is even or odd.

1) $k = 2m$. We have $\mathrm{res}^i_{\mathcal{A}}(T) \notin \{\varnothing, S\}$ for all $i = 1, \dots, m-1$ as otherwise $k = 2m$ would not be the minimum. We can apply Equation (38) and obtain

$$\mathrm{res}^{2(m-1)}_{\mathcal{B}}(T \cup \{\spadesuit\}) = \mathrm{res}^{m-1}_{\mathcal{A}}(T) \cup \{\spadesuit\}.$$

Applying Equation (35) to this result, we also obtain

$$\mathrm{res}_{\mathcal{B}}^{2(m-1)+1}(T \cup \{\spadesuit\}) = \mathrm{res}_{\mathcal{B}}^{2m-1}(T \cup \{\spadesuit\}) = S \setminus \mathrm{res}_{\mathcal{A}}^{m-1}(T) \cup \{\heartsuit\}.$$

Since $\varnothing \subsetneq \mathrm{res}_{\mathcal{A}}^{m-1}(T) \subsetneq S$, we have $\varnothing \subsetneq S \setminus \mathrm{res}_{\mathcal{A}}^{m-1}(T) \subsetneq S$, thus reaction (33) is not enabled by $(S \setminus \mathrm{res}_{\mathcal{A}}^{m-1}(T)) \cup \{\heartsuit\}$, implying in turn that $\heartsuit \notin \mathrm{res}_{\mathcal{B}}^{2m}(T \cup \{\spadesuit\})$, and thus $\mathrm{res}_{\mathcal{B}}^{2m}(T \cup \{\spadesuit\}) \neq S \cup \{\heartsuit, \spadesuit\}$. But since $\mathrm{res}_{\mathcal{B}}^{2m}(T \cup \{\spadesuit\}) \in \{\varnothing, S'\}$ then $\mathrm{res}_{\mathcal{B}}^{2m}(T \cup \{\spadesuit\}) = \varnothing$. Suppose now for a contradiction that $\mathrm{res}_{\mathcal{A}}^{m}(T) \neq \varnothing$: then it would also be $\mathrm{res}_{\mathcal{B}}^{2m}(T \cup \{\spadesuit\}) = \mathrm{res}_{\mathcal{B}}((S \setminus \mathrm{res}_{\mathcal{A}}^{m-1}(T)) \cup \{\heartsuit\}) \neq \varnothing$, a contradiction. We deduce that $\mathrm{res}_{\mathcal{A}}^{m}(T) = \varnothing$, thus T is attracted by $\{\varnothing, S\}$.

2) $k = 2m+1$. As before, $\mathrm{res}_{\mathcal{A}}^{i}(T) \notin \{\varnothing, S\}$ for $i = 1, \ldots, m-1$. Thus we have $\mathrm{res}_{\mathcal{B}}^{2m-1}(T \cup \{\spadesuit\}) = (S \setminus \mathrm{res}_{\mathcal{A}}^{m-1}(T)) \cup \{\heartsuit\}$. Since $\mathrm{res}_{\mathcal{B}}^{2m}(T \cup \{\spadesuit\}) = \mathrm{res}_{\mathcal{B}}^{k-1}(T \cup \{\spadesuit\}) \neq \varnothing$ then $\mathrm{res}_{\mathcal{A}}^{m}(T) \neq \varnothing$. Thus $\mathrm{res}_{\mathcal{B}}^{2m}(T \cup \{\spadesuit\}) = \mathrm{res}_{\mathcal{A}}^{m}(T) \cup \{\spadesuit\}$. Suppose for a contradiction that $\mathrm{res}_{\mathcal{A}}^{m}(T) \subsetneq S$, then, by Equation (35), $\mathrm{res}_{\mathcal{B}}^{2m+1}(T \cup \{\spadesuit\}) = S \setminus \mathrm{res}_{\mathcal{A}}^{m}(T) \cup \{\heartsuit\} \notin \{\varnothing, S'\}$, a contradiction by the definition of k. We deduce that $\mathrm{res}_{\mathcal{A}}^{m}(T) = S$, thus T is attracted by $\{\varnothing, S\}$.

Summing up, we proved that if $\{\varnothing, S'\}$ is a global attractor for $\mathcal{B}$ then $\{\varnothing, S\}$ is a global attractor for $\mathcal{A}$. ■

Claim 5, together with Claim 3, directly implies that there exists global 2-cycle attractor for $\mathcal{B}$ if and only if $\{\varnothing, S\}$ is a global attractor for $\mathcal{A}$. We also remark that the map $\mathcal{A} \mapsto \mathcal{B}$ can be constructed in polynomial time. By Theorem 17, deciding whether $\{\varnothing, S\}$ is a global attractor is **PSPACE**-complete, thus the thesis follows. □

6. Cycles of reactantless reaction systems

In this section, we prove **PSPACE**-hardness for problems concerning cycles in the class of reactantless RS. To this aim, we will reduce from the same problems studied in Section 4 for inhibitorless reaction systems. We start by recalling a result from [29] that will prove useful in showing that deciding whether a state is part of a cycle for inhibitorless RS is **PSPACE**-hard.

Lemma 31 *([29]). Let $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ be such that $\bigcup\{P_a : a \in A\} = S$ and $\mathrm{res}_{\mathcal{A}}(S) = S$. Then, there exists $\mathcal{B} = (S', A') \in \mathcal{RS}(0,1)$ such that, for any $T \subseteq S$, the following condition holds:*

$$\forall t \in \mathbb{N} \quad \mathrm{res}_{\mathcal{B}}^{2t}(T) = \mathrm{res}_{\mathcal{A}}^{t}(T) \quad \wedge \quad S \subseteq \mathrm{res}_{\mathcal{B}}^{2t+1}(T).$$

Furthermore, the map $\mathcal{A} \mapsto \mathcal{B}$ can be computed in polynomial time.

From now on we will follow the same reduction as in [29, Theorem 9].

Remark 32. Given any $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$ we can always construct another RS in $\mathcal{RS}(\infty, 0)$ having the same behaviour of $\mathcal{A}$ and satisfying the hypothesis of Lemma 31. Indeed, let $\mathcal{A}' = (S', A') \in \mathcal{RS}(\infty, 0)$ be such that $S' := S \cup \{\spadesuit\}$ for some $\spadesuit \notin S$, and $A' := A \cup \{(S', \varnothing, S')\}$. Therefore, since $(S', \varnothing, S') \in A'$ we have $\bigcup\{P'_a : a' \in A'\} = S'$ and $\mathrm{res}_{A'}(S') = S'$. Furthermore, $\mathrm{res}_{A}(T) = \mathrm{res}_{A'}(T)$ for all $T \subseteq S$.

Theorem 33. *Given $\mathcal{A} = (S, A) \in \mathcal{RS}(0, 1)$ and a state $T \subseteq S$, it is* **PSPACE***-complete to decide whether T is part of a cycle.*

Proof. The proof is entirely analogous to that of [29, Theorem 9]: we reduce from the problem of deciding whether T is part of a cycle in *inhibitorless* reaction systems.

Given $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$, we first construct another RS $\mathcal{A}' = (S', A') \in \mathcal{RS}(\infty, 0)$ from $\mathcal{A}$ using Remark 32; we then construct $\mathcal{A}'' \in \mathcal{RS}(0,1)$ from $\mathcal{A}'$ using Lemma 31. Notice that the map $\mathcal{A} \mapsto \mathcal{A}''$ can be computed in polynomial time.

Given a state $T \subseteq S$, we have $\mathrm{res}_{\mathcal{A}}^{t}(T) = T$ for some $t \in \mathbb{N}$ if and only if $\mathrm{res}_{\mathcal{A}''}^{2t}(T) = T$. Furthermore, it holds that $\mathrm{res}_{\mathcal{A}''}^{2s+1}(T) \neq T$ for all $s \in \mathbb{N}$, since $\spadesuit \in S' \subseteq \mathrm{res}_{\mathcal{A}''}^{2s+1}(T)$ but $\spadesuit \notin S$ and, in particular, $\spadesuit \notin T$. Therefore, T is part of a cycle in the RS $\mathcal{A}''$ if and only if the same happens in $\mathcal{A}$. Hence, by Theorem 20, deciding if T is part of a cycle for $\mathcal{RS}(0,1)$ is **PSPACE**-hard. □

Since $\mathcal{RS}(0,1)$ is a subclass of $\mathcal{RS}(0,\infty)$, we have the following result.

Corollary 34. *Given $\mathcal{A} = (S, A) \in \mathcal{RS}(0, \infty)$ and a state $T \subseteq S$, it is* **PSPACE***-complete to decide whether T is part of a cycle.*

The reduction of [29, Lemma 8], does not apply to the problems of sharing cycles, thus we need a new construction, provided in Theorem 35.

Theorem 35. *Given $\mathcal{A}, \mathcal{B} \in \mathcal{RS}(0, \infty)$ over the same background set S, it is* **PSPACE***-complete to decide if (1) $\mathcal{A}$ and $\mathcal{B}$ share all their cycles, and (2) $\mathcal{A}$ and $\mathcal{B}$ have a common cycle.*

Proof. Given $\mathcal{A} = (S, A) \in \mathcal{RS}(\infty, 0)$, we construct $\mathcal{A}' := (S', A') \in \mathcal{RS}(0, \infty)$, with $S' := S \cup \overline{S}$ where $\overline{S} := \{\overline{s} : s \in S\}$, i.e. the entities in $\overline{S}$ are in a one-to-one correspondence with those of S. In the following, given $T \subseteq S$ we denote by $\overline{T} := \{\overline{s} : s \in T\} \subseteq \overline{S}$. The following reactions give the set A':

$$\begin{aligned}
&(\varnothing, \{s\}, \{\overline{s}\}) && \text{for } s \in S \\
&a' := (\varnothing, \overline{R_a}, P_a) && \text{for } a = (R_a, \varnothing, P_a) \in A.
\end{aligned}$$

Clearly, $\mathcal{A}'$ is a reactantless reaction system. Given a state $V \cup \overline{U} \subseteq S'$, where $V \subseteq S$ and $\overline{U} \subseteq \overline{S}$, we notice that

$$\mathrm{res}_{\mathcal{A}'}(V \cup \overline{U}) = \mathrm{res}_{\mathcal{A}}(S \setminus U) \cup \overline{S \setminus V}, \tag{39}$$

since an entity $\overline{s} \in \overline{S}$ is generated if and only if $s \notin V$, and $a' \in A'$ is enabled if and only if $\overline{U} \cap \overline{R_a} = \varnothing \Leftrightarrow \overline{R_a} \subseteq \overline{S \setminus U} \Leftrightarrow R_a \subseteq S \setminus U$, i.e. the reaction $a \in A$ is enabled by $S \setminus U$. Furthermore, note that applying two times the reaction (39) to $V \cup \overline{S \setminus U}$, since $S \setminus (S \setminus V) = V$, we obtain:

$$\mathrm{res}^2_{\mathcal{A}'}\left(V \cup \overline{S \setminus U}\right) = \mathrm{res}_{\mathcal{A}}(V) \cup \overline{S \setminus \mathrm{res}_{\mathcal{A}}(U)} \tag{40}$$

Let now $\mathcal{B} = (S, B) \in \mathcal{RS}(\infty, 0)$ be over the same background set S as $\mathcal{A}$; we construct $\mathcal{B}' = (S', B') \in \mathcal{RS}(0, \infty)$ in much the same way as we did to construct $\mathcal{A}'$.

Claim 1. $\mathcal{A}, \mathcal{B}$ share all their cycles if and only if $\mathcal{A}', \mathcal{B}'$ share all their cycles.

$\boxed{\Rightarrow}$ Suppose $\mathcal{A}, \mathcal{B}$ share all their cycles and let $\left\{C_i \cup \overline{S \setminus D_i} \,:\, i \in \mathbb{Z}_k\right\}$ be a cycle for $\mathcal{A}'$, i.e. $\mathrm{res}_{\mathcal{A}'}\left(C_i \cup \overline{S \setminus D_i}\right) = C_{i+1} \cup \overline{S \setminus D_{i+1}}$ for all $i \in \mathbb{Z}_k$, where $i+1$ must be interpreted modulo k. From Equation (40), we get the following relations:

$$\forall i \in \mathbb{Z}_k, \quad C_{i+2} = \mathrm{res}_{\mathcal{A}}(C_i) \quad \text{and} \quad D_{i+2} = \mathrm{res}_{\mathcal{A}}(D_i)$$

and from Equation (39) we obtain that, for all $i \in \mathbb{Z}_k$, $C_{i+1} = \mathrm{res}_{\mathcal{A}}(D_i)$, thus $D_{i+2} = C_{i+1}$. Therefore we can rewrite the cycles as $\{C_i \cup \overline{S \setminus C_{i-1}} \,:\, i \in \mathbb{Z}_k\}$. We divide two cases:

(i) If k is even, then $C_0, C_2, \ldots, C_{k-2}$ and $C_1, C_3, \ldots, C_{k-1}$ are two cycles of $\mathcal{A}$. By hypothesis, they are also cycles of $\mathcal{B}$, therefore $\left\{C_i \cup \overline{S \setminus C_{i-1}} \,:\, i \in \mathbb{Z}_k\right\}$ is a cycle for $\mathcal{B}'$.

(ii) If k is odd, then $C_0, C_2, \ldots, C_{k-1}, C_1, C_3, \ldots, C_{k-2}$ is a cycle of $\mathcal{A}$, and we can conclude as in (i).

We thus proved that every cycle of $\mathcal{A}'$ is also a cycle of $\mathcal{B}'$. The same proof holds if we change the roles of $\mathcal{A}'$ and $\mathcal{B}'$, so we obtain the thesis.

$\boxed{\Leftarrow}$ Suppose $\mathcal{A}', \mathcal{B}'$ share all their cycles and let $\{E_i \,:\, i \in \mathbb{Z}_m\}$ be a cycle for $\mathcal{A}$. Consider the cycle in the dynamics of $\mathcal{A}'$ containing $E_0 \cup \overline{S \setminus E_0}$. This cycle is given by m blocks of the following type:

$$\cdots \to E_i \cup \overline{S \setminus E_i} \to E_{i+1} \cup \overline{S \setminus E_i} \to \cdots$$

for all $i \in \mathbb{Z}_m$. By hypothesis, this is also a cycle for $\mathcal{B}'$, therefore

$$\mathrm{res}_{\mathcal{B}'}\left(E_i \cup \overline{S \setminus E_i}\right) = E_{i+1} \cup \overline{S \setminus E_i} \quad \forall i \in \mathbb{Z}_m$$

and by Equation (39), we obtain that $E_{i+1} = \mathrm{res}_{\mathcal{B}}(E_i)$ for all $i \in \mathbb{Z}_m$, i.e. $\{E_i \,:\, i \in \mathbb{Z}_m\}$ is a cycle for $\mathcal{B}$. Therefore every cycle of $\mathcal{A}$ is also a cycle of $\mathcal{B}$. The same reasoning also holds if we exchange the roles of $\mathcal{A}$ and $\mathcal{B}$, so we obtain the thesis.

With similar reasoning as in Claim 1, it is also possible to prove the following claim.

Claim 2. $\mathcal{A}$ and $\mathcal{B}$ have a common cycle if and only if $\mathcal{A}'$ and $\mathcal{B}'$ have a common cycle.

We finally remark that the map $(\mathcal{A}, \mathcal{B}) \mapsto (\mathcal{A}', \mathcal{B}')$ can be constructed in polynomial time. By Theorems 21 and 22, the problems considered are **PSPACE**-hard for $\mathcal{RS}(\infty, 0)$, thus by Claims 1 and 2 the thesis follows. $\square$

7. Conclusions

We have provided a complete landscape of the complexity of problems related to the existence and identification of cycles and global attractors in reactantless and inhibitorless reaction systems. Specifically, we proved that the problems of deciding whether a given state is a global attractor and whether there exists a fixed point attractor in a given reaction system, which are **PSPACE**-complete in general reaction systems, become polynomial when they are restricted to the reactantless or inhibitorless case. Furthermore, again in contrast with the general case, no global cycle attractor of length at least 2 can exist in an inhibitorless RS, and no such a cycle of length strictly greater than 2 exists in a reactantless RS; and it is **PSPACE**-complete to decide whether a global cycle attractor of length exactly 2 exists in a reactantless RS. Finally, we proved that the problems of deciding if a state is part of a cycle and comparing the cycles of two reaction systems (do they have a common cycle? Do they have exactly the same cycles?) remain **PSPACE**-complete even when they are restricted to the inhibitorless and reactantless case. It remains open to study the complexity of the latter problems in the case of additive reaction systems, where we expect the hardness to reduce, as shown in [28] for other problems. Finding other classes besides additive reaction systems where those problems exhibit lower complexity is also of theoretical interest.

CRediT authorship contribution statement

Rocco Ascone: Writing – review & editing, Writing – original draft, Validation, Investigation, Formal analysis, Conceptualization. **Giulia Bernardini:** Writing – review & editing, Writing – original draft, Supervision. **Luca Manzoni:** Supervision, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

No data was used for the research described in the article.

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