Minimal Reaction Systems

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Abstract. Reaction systems are a formal model for processes inspired by the functioning of the living cell. These processes are determined by the iteration of the state transition functions of reaction systems, also called rs functions. In this paper we provide mathematical characterisations of rs functions implemented/defined by "minimal reaction systems", i.e., reaction systems with reactions using the minimal number of reactants, or the minimal number of inhibitors, or the minimal number of resources (i.e., reactants and inhibitors together).

Keywords: natural computing, functioning of the living cell, reaction, resources of reaction, reaction system, state transition function.

1 Introduction

Reaction systems, see, e.g., [3, 8, 9, 11–13] are a formal model for processes inspired by the functioning of the living cell. The central idea of this model is that the functioning of a living cell is based on interactions between individual reactions, and moreover these interactions are regulated by two main mechanisms: facilitation/acceleration and inhibition/retardation. These interactions determine the dynamic processes taking place in living cells, and reaction systems are an abstract model for such processes.

The formulation of the model of reaction systems based on the above principles takes into account the basic bioenergetics of the living cell. However, it remains a highly abstract model in the sense that it is not concerned with the quantitative details of the underlying chemistry of the living cell (stoichiometry, concentrations, etc.) but rather it is concerned with the understanding of processes carried out in the functioning living cell. Thus within the model of reaction systems one is not interested in the underlying "hardware/performance properties" of the living cell, but rather in the resulting processes. Consequently, there is no counting in the basic model of reaction systems — thus it is a qualitative rather than a quantitative model. Altogether, the above considerations yield a model that is quite different from the usual/standard models of computation.

The *framework of reaction systems* contains also models that are extensions of the basic model of reaction system. These extensions allow one to deal with

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various research topics — some of them allow the use of quantitative parameters. The research themes of this framework are motivated either by biological considerations or by the need to understand the underlying computations. They include among others:

- the notion of time in reaction systems, see [13];
- formation of modules (in the sense of [22]) in biological systems as modelled by reaction systems, see [11];
- investigation of decay of bio-entities and its influence on processes of the living cell (as modelled by reaction systems), see [5];
- static and dynamic causalities between entities, see [4];
- accounting for quantitative aspects through the use of so-called measurement functions, see [8, 13];
- mathematical understanding of state transition functions of reaction systems, see [3, 9, 10, 21].

This paper belongs to the last line of research from the above list. In particular, we provide mathematical characterisations of the state transition function of *minimal* reaction systems (i.e., reaction systems that operate with the minimal number of reactants, or the minimal number of inhibitors, or the minimal total number of resources, i.e., reactants and inhibitors together).

We refer the reader interested in a broader perspective of various formal models for bioprocesses to Section 3, at the end of which (after the model of reaction systems is formally introduced and discussed) we compare reaction systems with two well-established models, viz. process algebras and Petri nets.

2 Preliminaries

Throughout the paper we use standard mathematical notation. In particular, $\forall$ denotes the universal quantifier, $\exists$ the existential quantifier, $\varnothing$ the empty set, $X \setminus Y$ set difference, $X \cup Y$ set union, $X \cap Y$ set intersection, $X \subseteq Y$ set inclusion, and $2^X = \{Y : Y \subseteq X\}$ is the powerset of X. For a function $f : X \to Y$, $range(f) = \{y \in Y : (\exists x \in X)\ [f(x) = y]\}$. For a finite nonempty set S, a total function $f : 2^S \to 2^S$, and a nonempty $\mathcal{F} \subseteq 2^S$, we let

$$f(\mathcal{F}) = \{f(T) : T \in \mathcal{F}\} \text{ and } \bigcup \mathcal{F} = \bigcup_{T \in \mathcal{F}} T \text{ and } \bigcap \mathcal{F} = \bigcap_{T \in \mathcal{F}} T \ .$$

3 Reactions and Reaction Systems

In this section, we recall some key definitions concerning reactions and reaction systems (see, e.g., [3, 12]).

Definition 1. *Let S be a finite set (the* background *set of* entities*). A* reaction *over S is a triplet $a = (R, I, P)$, where $R, I, P \subseteq S$ are nonempty sets of entities such that $R \cap I = \varnothing$.*

The three component sets of reaction a are denoted by R_a, I_a and P_a, respectively, and called the set of *reactants*, the set of *inhibitors*, and the set of *products*. Also $R_a \cup I_a$ is called the set of *resources* of a, denoted by M_a. We use $rac(S)$ to denote the set of all reactions over S.

This formal notion of reaction has a clear biochemical intuition: a biochemical reaction may take place if all of its reactants are currently present and none of its inhibitors is currently present. This intuition leads to the definition of the effect of a set of reactions on a current state given below. Technically, we need to define first the effect of a single reaction.

Definition 2. *Let S be a finite set , let $T \subseteq S$, and let $a \in rac(S)$.*

(i) *a is* enabled *by T, denoted by $en_a(T)$, if $R_a \subseteq T$ and $I_a \cap T = \varnothing$.*

(ii) *The* result *of a on T is defined by*

$$res_a(T) = \begin{cases} P_a \text{ if } a \text{ is enabled by } T \\ \varnothing \quad \text{otherwise} . \end{cases}$$

The result of a set of reactions A on a current state is cumulative i.e., it is the union of results of all individual reactions from A.

Definition 3. *Let S be a finite set, let $T \subseteq S$, and let $A \subseteq rac(S)$. The* result *of A on T, denoted by $res_A(T)$, is defined by*

$$res_A(T) = \bigcup \{res_a(T) : a \in A\} .$$

In the above, the finite set T formalises a state of a biochemical system (e.g., the cell), i.e., the set of biochemical entities currently present in it. Thus if transitions from the current state to its successor are determined only by the enabled reactions (i.e., there is no influence by the environment), then the successor state consists only of the entities produced by the enabled reactions. This implies that there is *non-permanency*: in the transition from a current state T to its successor, an *entity from T vanishes unless it is sustained by a reaction.* This assumption/property reflects the basic bioenergetics of the living cell: without flow/supply of energy the living cell disintegrates, but the use/absorption of energy by the living cell is achieved through biochemical reactions (see, e.g., [19]).

Note that if a and b are two reactions from A enabled by T, then $P_a \cup P_b \subseteq res_A(T)$, even if $R_a \cap R_b \neq \varnothing$. This means that we do not have the notion of conflict between reactions if they need to share reactants. This follows from the assumption of the *threshold nature of resources*: either an entity is available and then there is "enough of it", or it is not available. This in turn reflects the *level of abstraction* adopted for the formulation of the basic model: one does not count concentrations of entities/molecules to infer from these which reactions can/will be applied. The model operates on a higher level of abstraction: one assumes that the cell is running/functioning and the goal is to understand the processes going on. At this stage, one is not interested in the underlying "hardware/performance

properties" of the living cell, but rather in the resulting processes. Consequently, there is no counting in the basic model, and so we deal with a *qualitative* rather than with a *quantitative* model (thus technically, we deal with sets rather than, e.g., with multisets). This is a basic difference with the traditional models of concurrent systems in computer science, such as, e.g., Petri nets (see, e.g., [7, 18]). This non-counting assumption holds for the basic model of reaction systems. However, in the more general framework of reaction systems one also admits models that allow counting, see, e.g., [8, 13].

We are now ready to define reaction systems.

Definition 4. *A* reaction system*, abbreviated rs, is an ordered pair* $\mathcal{A} = (S, A)$*, where* S *is a finite set and* $A \subseteq rac(S)$*.*

The set S is called the *background set* of $\mathcal{A}$, and its elements are called the *entities* of $\mathcal{A}$ — they represent molecular entities (e.g., atoms, ions, molecules) that may be present in the states of the biochemical system (e.g., the living cell). The set A is called the set of *reactions of* $\mathcal{A}$; clearly A is finite (as S is finite).

The subsets of S are called the *states of* $\mathcal{A}$. Given a state $T \subseteq S$, the *result of* $\mathcal{A}$ on T, denoted by $res_{\mathcal{A}}(T)$, is defined by $res_{\mathcal{A}}(T) = res_A(T)$.

Thus a reaction system is essentially a set of reactions. The specification of a reaction system $\mathcal{A}$ includes also its background set S, which is such that all reactions of $\mathcal{A}$ are over S. There are no "structures" involved in reaction systems (such as, e.g., the tape of a Turing machine, [17]). It is important to note that this is a *strictly finite model* — its size is restricted by the size of its background set.

We end this section by briefly discussing the relationship of reaction systems to two well established models of bioprocesses: process algebras (in the form they are applied to bioprocesses) and Petri nets (in the form they are applied to bioprocesses), providing in this way the reader with a more general perspective on the broad research area where this paper belongs.

We begin by comparing reaction systems with process algebras (see, e.g., [20], [6] and [2]).

(1) First of all, reaction systems are a "model from scratch" — it resulted from stating a number of key properties of the functioning of the living cell (where the functioning is determined by interactions between chemical reactions), determining the level of abstraction, and then formulating accordingly the model. The model is basically a finite set of reactions, where the notions of a reaction, applicability (enabling) of a set of reactions, the result of applying reactions to a current state, and the notion of a process reflect/formalise the key properties mentioned above (see, e.g., [3]).

The process algebra approach to modelling bioprocesses is based on a long existing and well established research field of process algebra. The clear advantage is the existence of a great body of knowledge about, and software tools for process algebras.

(2) The model of reaction systems is a foundational model which is aimed at providing general theory of modelled reality, i.e., formulating general notions

(such as time, decay, formation of modules, etc) and then proving general properties of modelled reality using these notions.

Modelling of biological processes with process algebra concentrates mainly on simulation of (a whole range of) specific cases and in this sense it is more application oriented than reaction systems.

(3) The basic model of reaction systems is deterministic while process algebras used in bio-modelling are stochastic. It is instructive to point out here that reaction systems allow also for defining nondeterministic and stochastic processes (see, e.g., [3], [8] and [16]).

(4) The basic model of reaction systems is qualitative (and the standard notion of conflict does not exist here) while the model of process algebra used in bio-modelling is quantitative. Again, it is instructive to add here that counting (adding numerical parameters to states) has been accommodated in the broader framework of reaction systems (see, e.g., [8] and [13]).

(5) The model of reaction systems is *strictly* finite (as the background set is finite). Hence, e.g., all states in all processes have an *a priori* bounded cardinality. This is not true for process algebra where, e.g., one can get an unbounded increase of individuals of a given species, and consequently the number of components in a parallel composition of processes is not a priori bounded.

(6) A key technical feature of reaction systems is *non-permanency*: the only entities present in the successor state T' of a current state T are the entities produced by reactions enabled by T (or, in a context-dependent process, entities added by the context of T').

This feature does not hold for process algebras, where processes not activated in a current state will just carry over to the successor state.

The comparison of reaction systems with Petri as used for modelling of bio-processes (see, e.g., [1, 14, 15]) yields quite similar conclusions. Following the points stated above: (1) holds also for Petri nets; (2) also holds, although some general properties of Petri nets (invariants, deadlocks, traps) get a direct interpretation in modelled biological systems; (3) also here, nondeterministic and stochastic features of Petri nets are essential for modelling of biological systems; (4) modelling of bioprocesses is mostly based on quantitative parameters, although some research pursues a qualitative analysis (but even there conflict plays a major role); (5) holds also for majority of research here (there is no a priori bound on the number of states/markings); (6) the non-permanency feature does not hold for Petri nets, tokens from the current marking/state not involved in enabled transitions remain present in the successor marking/state.

We would like to point out that there is a confusion concerning the term "qualitative" here: in "bio Petri nets" this term refers to Petri nets which are time-free. Hence the classical Petri nets will be called "qualitative" (!) while for us "qualitative" means that there is no counting.

4 Functions Defined by Reaction Systems

The model of reaction systems formalises the "static structure" of the living cell as the set of all reactions of the cell (together with the underlying entities). The

dynamic behaviour of the living cell is then formalised through the definition of processes.

The general definition of processes includes also (through so-called "contexts") the interaction with environment, see, e.g., [3, 12], taking into account the fact that the living cell is an open system. In the special case of "context-independent" processes, corresponding to considering the living cell as a closed-system (with no influence by the environment), the processes are determined/driven only by the iteration of the result function of a given rs.

In either case, the understanding of the properties of result functions is central to the understanding of the behaviour (state transitions) of reaction systems. This paper is concerned with properties of result functions specified/defined by the so-called "minimal" reaction systems. In this section we define some central notions concerning these functions.

Definition 5. *Let S be a finite nonempty set.*

(i) *For an rs $\mathcal{A}$ we say that $\mathcal{A}$* implements *$res_{\mathcal{A}}$.*

(ii) *A function $f : 2^S \to 2^S$ is an* rs-function *if there exists an rs $\mathcal{A}$ such that $f = res_{\mathcal{A}}$.*

Note that for an rs $\mathcal{A}$ with background set S, $res_{\mathcal{A}}(\varnothing) = \varnothing$, as the set of reactants for every reaction is nonempty and so no reaction is enabled by $\varnothing$. Similarly, $res_{\mathcal{A}}(S) = \varnothing$, as the set of inhibitors for every reaction is nonempty and so no reaction is enabled by S. It was proved in [12] that these two "boundary conditions" characterise rs functions.

Proposition 1 ([12]). *Let S be a finite nonempty set. A function $f : 2^S \to 2^S$ is an rs function iff $f(\varnothing) = f(S) = \varnothing$.*

Our main interest in the line of research represented by this paper is to understand the nature of rs functions. Therefore, we call two rs systems, $\mathcal{A}_1$ and $\mathcal{A}_2$, with the same background set *equivalent* if $res_{\mathcal{A}_1} = res_{\mathcal{A}_2}$; we write then $\mathcal{A}_1 \sim \mathcal{A}_2$. Thus two equivalent reaction systems represent two different implementations of the same rs function.

In this paper we will investigate rs functions implementable by "minimal reaction systems" which are defined as follows.

Definition 6. *Let $\mathcal{A} = (S, A)$ be an rs.*

(i) *$\mathcal{A}$ is* reactant-minimal *if* $|R_a| = 1$ *for each $a \in A$.*

(ii) *$\mathcal{A}$ is* inhibitor-minimal *if* $|I_a| = 1$ *for each $a \in A$.*

(iii) *$\mathcal{A}$ is* resource-minimal *if* $|M_a| = 2$ *for each $a \in A$.*

Clearly, $\mathcal{A}$ is resource-minimal if and only if it is both reactant-minimal and inhibitor-minimal.

This classification carries over to rs functions as follows.

Definition 7. *Let S be a finite nonempty set, and let $f : 2^S \to 2^S$ be an rs function.*

(i) f *is* reactant-minimal *if there is a reactant-minimal rs implementing* f.
(ii) f *is* inhibitor-minimal *if there is an inhibitor-minimal rs implementing* f.
(iii) f *is* resource-minimal *if there is a resource-minimal rs implementing* f.

Clearly, if f is resource-minimal then it is both reactant-minimal and inhibitor-minimal.

We end this section by defining two notions used throughout this paper.

Definition 8. *Let* S *be a finite set, and* f *be a function* $f : 2^S \to 2^S$.

(i) f *is* union-subadditive *if* $(\forall X, Y \subseteq S)\,[\, f(X \cup Y) \subseteq f(X) \cup f(Y)\,]$.
(ii) f *is* intersection-subadditive *if* $(\forall X, Y \subseteq S)\,[\, f(X \cap Y) \subseteq f(X) \cup f(Y)\,]$.

The following are examples of functions over a set $S = \{a, b, c\}$ that are respectively not union-subadditive and not intersection-subadditive:

$$\begin{array}{lll} f(\{a\}) = \{a\} & f(\{b\}) = \{b\} & f(\{a,b\}) = \{c\} \\ g(\{a,b\}) = \{b\} & g(\{a,c\}) = \{c\} & g(\{a\}) = \{a\} \end{array}$$

Since we always deal with finite background sets, the following technical result applies.

Lemma 1. *Let* S *be a finite set and* f *be a function* $f : 2^S \to 2^S$.

(i) f *is union-subadditive iff* $(\forall \mathcal{F} \subseteq 2^S, \mathcal{F} \neq \varnothing)\,[\, f\big(\bigcup \mathcal{F}\big) \subseteq \bigcup f(\mathcal{F})\,]$.
(ii) f *is intersection-subadditive iff* $(\forall \mathcal{F} \subseteq 2^S, \mathcal{F} \neq \varnothing)\,[\, f\big(\bigcap \mathcal{F}\big) \subseteq \bigcup f(\mathcal{F})\,]$.

Proof. Follows from S being finite. □

5 Reactant-Minimal rs Functions

In this section we provide a characterisation of reactant-minimal rs functions. We begin with a technical result which will be useful in the proof of the characterisation theorem (Theorem 1).

Proposition 2. *Let, for a finite set* S, $f : 2^S \to 2^S$ *be a union-subadditive function. Then:*

$$(\forall T \subseteq S, T \neq \varnothing)(\forall q \in f(T))(\exists x \in T)(\forall U \subseteq T)\;[\, x \in U \implies q \in f(U)\,]\,.$$

Proof. By contradiction. Assume that the proposition does not hold. Then:

$$(\exists T_0 \subseteq S, T_0 \neq \varnothing)(\exists q_0 \in f(T_0))(\forall x \in T_0)(\exists U \subseteq T_0) \\ [\, x \in U \text{ and } q_0 \notin f(U)\,]\,. \qquad (*)$$

In the above, U is not necessarily unique for a given x, but for each $x \in T_0$ we choose one such set and denote it by U_x .

Let $\mathcal{F} = \{U_x : x \in T_0\}$. We note that:

(i) $\bigcup \mathcal{F} = T_0$ by $(\forall x \in T_0)\ [\, x \in U_x \subseteq T_0 \,]$.
(ii) $q_0 \in f(T_0)$ by $(*)$.
(iii) $(\forall x \in T_0)\ [\, q_0 \notin f(U_x) \,]$ by $(*)$.
(iv) $q_0 \in f\big(\bigcup \mathcal{F}\big)$ by (i).
(v) $q_0 \notin \bigcup\{f(U_x) : x \in T_0\}$ by (iii).

We then observe from the definition of $\mathcal{F}$ that (iv) and (v) together are in contradiction with the assumption that f is union-subadditive (see Lemma 1). Therefore $(*)$ does not hold and so the proposition holds. □

Theorem 1. *Let, for a finite nonempty set S, $f : 2^S \to 2^S$ be an rs function. Then the following statements are equivalent:*

(α) f is reactant-minimal.
(β) f is union-subadditive.

Proof (Theorem 1). The proof consists of two parts which, when combined, will constitute the proof of the equivalence of the two statements in the formulation of this theorem.

Part 1. $(\alpha) \Longrightarrow (\beta)$.

Proof (Part 1). Let $\mathcal{A} = (S, A)$ be a reactant-minimal rs implementing f.

Let $T, U \subseteq S$ be such that $res_{\mathcal{A}}(T \cup U) \neq \varnothing$. Let $q \in res_{\mathcal{A}}(T \cup U)$. Then there exists $a \in A$ such that $en_a(T \cup U)$ and $q \in P_a$.

Since $\mathcal{A}$ is reactant-minimal, $R_a = \{x\}$ for some $x \in S$. Since $en_a(T \cup U)$, $x \in T \cup U$ and $I_a \cap (T \cup U) = \varnothing$. Thus $x \in T$ or $x \in U$, and moreover $I_a \cap T = \varnothing$ and $I_a \cap U = \varnothing$. Consequently, if $x \in T$, then $en_a(T)$, and if $x \in U$, then $en_a(U)$. If the former holds then $q \in res_{\mathcal{A}}(T)$, and if the latter holds, then $q \in res_{\mathcal{A}}(U)$. Thus $q \in res_{\mathcal{A}}(T) \cup res_{\mathcal{A}}(U)$.

Hence $q \in res_{\mathcal{A}}(T \cup U)$ implies $q \in res_{\mathcal{A}}(T) \cup res_{\mathcal{A}}(U)$. Consequently, we obtain that:

$$res_{\mathcal{A}}(T \cup U) \subseteq res_{\mathcal{A}}(T) \cup res_{\mathcal{A}}(U)\ .$$

Also, if $res_{\mathcal{A}}(T \cup U) = \varnothing$, then $res_{\mathcal{A}}(T \cup U) \subseteq res_{\mathcal{A}}(T) \cup res_{\mathcal{A}}(U)$. Hence $f = res_{\mathcal{A}}$ is union-subadditive. Thus assuming (α) we get (β). This concludes the first part of the proof. *(Part 1)* □

Part 2. $(\beta) \Longrightarrow (\alpha)$.

Proof (Part 2). Assume that (β) holds. We will show that then f is reactant-minimal. For all $T \subseteq S$ and $q \in f(T)$, we select one $x \in T$ satisfying the statement of Proposition 2 and denote it by x_T^q. Let now a_T^q be the reaction $(\{x_T^q\}, S \setminus T, \{q\})$ — note that if $T \in \{\varnothing, S\}$, then, since f is a rs function, $f(T) = \varnothing$ and so neither x_T^q nor a_T^q are defined. Let then $\mathcal{A} = (S, A)$ be the reaction system with:

$$A = \{a_T^q : T \subseteq S \text{ and } q \in f(T)\}\ .$$

Claim 1. *$\mathcal{A}$ is reactant-minimal.*

Proof (Claim 1). Directly from the definition of $\mathcal{A}$. *(Claim 1)* □

Claim 2. *$res_{\mathcal{A}} = f$.*

Proof (Claim 2). We first show that:

$$(\forall T \subseteq S)\ [\, f(T) \subseteq res_{\mathcal{A}}(T)\,]\,. \qquad (*)$$

Let $T \subseteq S$ and $q \in f(T)$. By the construction of $res_{\mathcal{A}}$,

$$a^q_T = (\{x^q_T\}, S \setminus T, \{q\}) \in A\,.$$

Since $x^q_T \in T$, a^q_T is enabled by T. Therefore, by the definition of x^q_T, we have $q \in res_{\mathcal{A}}(T)$. Consequently, $f(T) \subseteq res_{\mathcal{A}}(T)$, and so $(*)$ holds.

We next show that

$$(\forall T \subseteq S)\ [\, res_{\mathcal{A}}(T) \subseteq f(T)\,]\,. \qquad (**)$$

Let $T \subseteq S$ and $q \in res_{\mathcal{A}}(T)$. Hence:

$$(\exists a \in A)\ [\, en_a(T) \text{ and } q \in P_a\,]\,.$$

Note that this a does not have to be a^q_T. However, since $a \in A$, $a = a^q_W$, for some $W \subseteq S$ and so $a = (\{x^q_W\}, S \setminus W, \{q\})$. We note that:

(i) $T \subseteq W$.
Otherwise $\exists y \in T \cap (S \setminus W)$, hence $y \in T \cap I_a$ which contradicts the fact that $en_a(T)$.

(ii) $x^q_W \in T$.
Because a is enabled by T.

(iii) $q \in f(T)$.
Because $P_a = \{q\}$.

Consequently, $res_{\mathcal{A}}(T) \subseteq f(T)$ and so $(**)$ holds. The claim then follows from $(*)$ and $(**)$. *(Claim 2)* □

By Claim 1 and Claim 2 it follows that f is reactant-minimal. Consequently, assuming (β) we get (α). This concludes Part 2 of the proof. *(Part 2)* □

Part 1 and Part 2 together imply that the theorem holds. *(Theorem 1)* □

6 Inhibitor-Minimal rs Functions

In this section we provide a characterisation theorem for inhibitor-minimal rs functions. The following technical notion will be useful in the proof of this theorem.

Let f be an rs function over S, $T \subseteq S$, $y \in S \setminus T$ and $q \in f(T)$. Then y is *f-excluding for T, q* if:

$$(\forall U \subseteq S)\ [\, (T \subseteq U \text{ and } y \notin U) \Longrightarrow q \in f(U)\,]\,.$$

We use $excluding(f, T, q)$ to denote the set of f-excluding entities for T, q.

Theorem 2. *Let, for a finite nonempty set S, $f : 2^S \to 2^S$ be an rs function. Then the following statements are equivalent:*

(γ) f is inhibitor-minimal.

(δ) f is intersection-subadditive.

Proof (Theorem 2). Again, as was the case with Theorem 1, the proof consists of two parts.

Part 1. $(\gamma) \Longrightarrow (\delta)$.

Proof (Part 1). Assume that (γ) holds, i.e., there is an inhibitor-minimal reaction system $\mathcal{A} = (S, A)$ such that $\mathcal{A}$ implements f. We will now show that then f is intersection-subadditive.

Let $\mathcal{F} \subseteq 2^S$ be nonempty and let $q \in f(\cap\mathcal{F})$. Then $q \in res_{\mathcal{A}}\big(\bigcap \mathcal{F}\big)$ and so:

$$(\exists a \in A)\ [\, a = (R_a, \{y\}, P_a) \text{ with } y \in S \setminus R_a,\ q \in P_a,\ \text{and } en_a\big(\bigcap \mathcal{F}\big)\,] \,.$$

Hence $R_a \subseteq \bigcap \mathcal{F}$ and $y \notin \bigcap \mathcal{F}$. Since $y \notin \bigcap \mathcal{F}$, we have $(\exists T \in \mathcal{F})\ [\, y \notin T\,]$; let T_0 be such a set in $\mathcal{F}$. Since $R_a \subseteq \bigcap \mathcal{F}$, we have $R_a \subseteq T_0$. Therefore T_0 enables a, and so $q \in res_{\mathcal{A}}(T_0)$. Hence

$$q \in \bigcup_{V \in \mathcal{F}} res_{\mathcal{A}}(V) = \bigcup res_{\mathcal{A}}(\mathcal{F}) \,.$$

Thus $res_{\mathcal{A}}\big(\bigcap \mathcal{F}\big) \subseteq \bigcup res_{\mathcal{A}}(\mathcal{F})$. Since $res_{\mathcal{A}} = f$, we get $f(\bigcap \mathcal{F}) \subseteq \bigcup f(\mathcal{F})$. Thus f is intersection-subadditive and so (δ) holds for f. Consequently, assuming (γ) we get (δ). This concludes Part 1 of the proof. *(Part 1)* □

Part 2. $(\delta) \Longrightarrow (\gamma)$.

Proof (Part 2).

Claim 3. $(\forall T \subseteq S)(\forall q \in f(T))(\exists y \in S \setminus T)\ [\, y \in \mathit{excluding}(f, T, q)\,]$.

Proof (Claim 3). By contradiction. Assume that the claim does not hold. Then:

$$(\exists T \subseteq S)(\exists q \in f(T))(\forall y \notin T)(\exists W \subseteq S) \\ [\, T \subseteq W \text{ and } y \notin W \text{ and } q \notin f(W)\,] \,.$$

In the above, W is not necessarily unique for a given y, but for each $y \notin T$ we choose one such set and denote it by W_y.
Note that, since $y \notin W_y$, we have $\bigcap_{y \notin T} W_y = T$. Hence, since $q \in f(T)$, we have:

$$q \in f\big(\bigcap_{y \notin T} W_y\big) \,. \qquad (*)$$

Moreover, since $(\forall y \notin T)\ [\, q \notin f(W_y)\,]$, we have:

$$q \notin \bigcup_{y \notin T} f(W_y) \,. \qquad (**)$$

From $(*)$ and $(**)$ we get

$$f\big(\bigcap_{y \notin T} W_y\big) \not\subseteq \bigcup_{y \notin T} f(W_y) \,.$$

This, however, contradicts the assumption that f is intersection-subadditive. Hence the claim holds. *(Claim 3)* □

We will now construct a reaction system $\mathcal{A}$ satisfying (γ). Let $\mathcal{A} = (S, A)$, where

$$A = \{(T, \{y\}, \{q\}) : T \subseteq S,\ q \in f(T) \text{ and } y \in \mathit{excluding}(f, T, q)\}\ .$$

Clearly, $\mathcal{A}$ is inhibitor-minimal. We will also prove that $\mathcal{A}$ implements f.

Claim 4. $(\forall T \subseteq S)\ [\, f(T) \subseteq \mathit{res}_{\mathcal{A}}(T)\,]$.

Proof (Claim 4). Let $T \subseteq S$ and $q \in f(T)$. Then:

$$(\exists a = (T, \{y\}, \{q\}) \in A)\ [\, y \in \mathit{excluding}(f, T, q)\,] \qquad (***)$$

which follows from Claim 3 (the existence of y being f-excluding for T, q), and the construction of $\mathcal{A}$. The reaction a in $(***)$ is enabled by T which follows from the definition of $y \in \mathit{excluding}(f, T, q)$. Hence $q \in \mathit{res}_{\mathcal{A}}(T)$.

Thus $q \in f(T)$ implies $q \in \mathit{res}_{\mathcal{A}}(T)$ and, as a consequence, $f(T) \subseteq \mathit{res}_{\mathcal{A}}(T)$. Hence the claim holds. *(Claim 4)* □

Claim 5. $(\forall V \subseteq S)\ [\, \mathit{res}_{\mathcal{A}}(V) \subseteq f(V)\,]$.

Proof (Claim 5). Let $V \subseteq S$ and $q \in \mathit{res}_{\mathcal{A}}(V)$. Then:

$$(\exists a \in A)\ [\, \mathit{en}_a(V) \text{ and } P_a = \{q\}\,]\ .$$

From the construction of $\mathcal{A}$ it then follows that this a is of the form $a = (T, \{y\}, \{q\})$, for some $T \subseteq V$ and $y \notin V$. Since $y \in \mathit{excluding}(f, T, q)$ and $y \notin V$, we get $q \in f(V)$. Hence $\mathit{res}_{\mathcal{A}}(V) \subseteq f(V)$. *(Claim 5)* □

Since $\mathcal{A}$ is an inhibitor-minimal reaction system, from Claim 4 and Claim 5 it follows that (γ) holds. Thus, assuming (δ) we get (γ). This concludes Part 2 of the proof. *(Part 2)* □

Part 1 and Part 2 together imply that the theorem holds. *(Theorem 2)* □

7 Resource-Minimal Focus rs Functions

We consider now minimality of the whole set of resources, i.e., the minimal total number of resources (reactants and inhibitors). The reader is referred to [10], where it is demonstrated that (iterations of) rs functions with minimal resources can generate quite "sophisticated" processes.

We will provide a characterisation of rs functions implementable with a minimal number of resources. This is done in two steps: first (in this section) we will consider only the so-called focus rs functions, and then (in the next section), we will consider arbitrary rs functions (using the characterisation result for focus rs functions). We begin by defining focus functions.

Definition 9. *A function $f : 2^S \to 2^S$ is a* focus function *if*

$$(\exists q \in S)\ [\, \mathit{range}(f) = \{\varnothing, \{q\}\}\,]\ .$$

This q, unique for f, is referred to as the focus of f.

We introduce now three technical notions which will be useful in the proofs of this section.

Let f be a focus function, $T \subseteq S$ and $x, y \in S$. Then:

(i) T is *focused by* f if

$$f(T) \neq \varnothing \, .$$

We use $\mathit{focused}(f)$ to denote the set of all $T \subseteq S$ focused by f.

(ii) x is *f-special* for T if $x \in T$ and

$$(\forall U \subseteq T)\, [\, x \in U \implies f(U) \neq \varnothing \,] \, .$$

We use $\mathit{special}(f, T)$ to denote the set of all $x \in T$ which are f-special for T.

(iii) y is an *f-partner of* x if $y \neq x$ and

$$(\forall U \subseteq S)\, [\, (x \in U \text{ and } y \notin U) \implies f(U) \neq \varnothing \,] \, .$$

We use $\mathit{partner}(f, x)$ to denote the set of all y which are f-partners of x.

We are now ready to prove a characterisation theorem for focus rs functions.

Theorem 3. *Let, for a finite nonempty set S, $f : 2^S \to 2^S$ be a focus function. Then the following statements are equivalent:*

(ζ) *f is resource-minimal.*

(η) *f is both union- and intersection-subadditive.*

Proof (Theorem 3). Let $q \in S$ be the focus of f. The proof will be delivered in two parts which together provide a proof of the equivalence of the two statements in the formulation of this proposition.

Part 1. (ζ) $\implies$ (η).

Proof (Part 1). Assume that (ζ) holds for f; hence there exists a resource-minimal reaction system $\mathcal{A}$ such that $\mathit{res}_{\mathcal{A}} = f$.

Claim 6. $(\forall \mathcal{F} \subseteq 2^S, \mathcal{F} \neq \varnothing)\ f\big(\bigcup \mathcal{F}\big) \subseteq \bigcup f(\mathcal{F})$.

Proof (Claim 6). We consider two cases.

Case 1: $f\big(\bigcup \mathcal{F}\big) = \varnothing$. Then, trivially, the claim holds.

Case 2: $f\big(\bigcup \mathcal{F}\big) = \{q\}$. Then, since $f = \mathit{res}_{\mathcal{A}}$, we have:

$$(\exists a = (\{x\}, \{y\}, \{q\}) \in A)\, [\, \mathit{en}_a\big(\bigcup \mathcal{F}\big) \,] \, .$$

Thus $x \in \bigcup \mathcal{F}$ and $y \notin \bigcup \mathcal{F}$, and consequently

$$(\exists T \in \mathcal{F})\, [\, x \in T \text{ and } y \notin T \,] \, .$$

Any such T enables a, and so $q \in res_{\mathcal{A}}(T) = f(T)$. Consequently $q \in \bigcup_{X \in \mathcal{F}} f(X)$. Thus:

$$f\big(\bigcup \mathcal{F}\big) = \{q\} \subseteq \bigcup f(\mathcal{F}) = \{q\} \ ,$$

and so the claim holds. *(Claim 6)* □

Claim 7. $(\forall \mathcal{F} \subseteq 2^S, \mathcal{F} \neq \varnothing)\ [\, f\big(\bigcap \mathcal{F}\big) \subseteq \bigcup f(\mathcal{F})\,]$.

Proof (Claim 7). We consider two cases.

Case 1: $f\big(\bigcap \mathcal{F}\big) = \varnothing$. Then, trivially, the claim holds.

Case 2: $f\big(\bigcap \mathcal{F}\big) = \{q\}$. Then, since $f = res_{\mathcal{A}}$, we have:

$$(\exists a = (\{x\}, \{y\}, \{q\}) \in A)\ [\, en_a\big(\bigcap \mathcal{F}\big)\,] \ .$$

Hence $x \in \bigcap \mathcal{F}$ and $y \notin \bigcap \mathcal{F}$.
This implies that:

$$(\exists T \in \mathcal{F})\ [\, x \in T \text{ and } y \notin T\,] \ .$$

Thus $(\exists T \in \mathcal{F})\ [\, en_a(T)$ and $q \in res_{\mathcal{A}}(T)\,]$.
Consequently $q \in \bigcup f(\mathcal{F})$, and so:

$$f\big(\bigcap \mathcal{F}\big) = \{q\} \subseteq \bigcup f(\mathcal{F}) = \{q\} \ .$$

Thus the claim holds. *(Claim 7)* □

From Claim 6 (f is union-subadditive) and Claim 7 (f is intersection-subadditive) it follows that $f = res_{\mathcal{A}}$ satisfies (η). Thus the assumption that (ζ) holds implies that (η). This concludes Part 1 of the proof. *(Part 1)* □

Part 2. $(\eta) \implies (\zeta)$.

Proof (Part 2). Assuming (η) means that:

$$(\forall \mathcal{F} \subseteq 2^S, \mathcal{F} \neq \varnothing)\ \big[\, f\big(\bigcup \mathcal{F}\big) \subseteq \bigcup f(\mathcal{F}) \text{ and } f\big(\bigcap \mathcal{F}\big) \subseteq \bigcup f(\mathcal{F})\,\big] \ .$$

Claim 8. $(\forall T \subseteq S, \mathcal{F} \neq \varnothing)\,[\, T \in \mathit{focused}(f) \implies (\exists x \in T)\,[\, x \in \mathit{special}(f, T)\,]\,]$.

Proof (Claim 8). By contradiction. Assume that the claim does not hold. Then:

$$(\exists T \subseteq S)\ [T \in \mathit{focused}(f) \text{ and } (\forall x \in T)(\exists U \subseteq T)[\, x \in U \text{ and } f(U) = \varnothing\,]]\,.$$

In the above, U is not necessarily unique for a given x, but for each $x \in T$ we choose one such set and denote it by U_x .
Since

$$(\forall x \in T)\ [\, x \in U_x \text{ and } U_x \subseteq T\,] \ ,$$

we have $T = \bigcup_{x \in T} U_x$, and since T is focused by f, we have:

$$f\big(\bigcup_{x \in T} U_x\big) = f(T) = \{q\} \ .$$

But since $(\forall x \in T)\ [f(U_x) = \varnothing]$, we get $\bigcup_{x \in T} f(U_x) = \varnothing$. Consequently, we obtain that:

$$f\big(\bigcup_{x \in T} U_x\big) = \{q\} \not\subseteq \bigcup_{x \in T} f(U_x) = \varnothing \ .$$

Thus f is not union-subadditive, which contradicts the assumption that (η) holds.

Thus the claim must hold. *(Claim 8)* □

Claim 9. $(\forall T \subseteq S)(\forall x \in S)\ [\,(T \in \mathit{focused}(f)\ \mathit{and}\ x \in \mathit{special}(f,T)) \implies (\exists y \notin T)\ [\,y \in \mathit{partner}(f,x)\,]]$.

Proof (Claim 9). By contradiction. Assume that the claim does not hold. Then

$$(\exists T \subseteq S)(\exists x \in T)\ [\,(T \in \mathit{focused}(f) \text{ and } x \in \mathit{special}(f,T)) \text{ and } (\forall y \notin T)\ (\exists W \subseteq S)[\,x \in W \text{ and } y \notin W \text{ and } f(W) = \varnothing\,]] \ .$$

In the above, W is not necessarily unique for a given y, but for each $y \notin T$ we choose one such set and denote it by W_y.

This assumption implies that:

(i)	$\bigcap_{y \notin T} W_y \subseteq T$	by $(\forall y \notin T)\ [\,y \notin W_y]$.
(ii)	$x \in \bigcap_{y \notin T} W_y$	by $(\forall y \notin T)\ [\,x \in W_y\,]$.
(iii)	$f\big(\bigcap_{y \notin T} W_y\big) = \{q\}$	by (i) and (ii), because $x \in \mathit{special}(f,T)$.
(iv)	$\bigcup_{y \notin T} f(W_y) = \varnothing$	by $(\forall y \notin T)\ [\,f(W_y) = \varnothing\,]$.

Then (iii) and (iv) imply that:

$$f\big(\bigcap_{y \notin T} W_y\big) = \{q\} \not\subseteq \bigcup_{y \notin T} f(W_y) = \varnothing \ .$$

Thus f is not intersection-subadditive, which contradicts (η).

Hence the claim holds. *(Claim 9)* □

To summarise, Claim 8 states that each f-focused subset T of S has an f-special element and Claim 9 states that each f-special element has an f-partner. We will now use these claims to prove that (ζ) holds for f. To this aim we construct $\mathcal{A} = (S, A)$ satisfying (ζ). Let

$$A = \{(\{x\},\{y\},\{q\}) : x, y \in S \text{ and } (\exists T \subseteq S)[\,x \in \mathit{special}(f,T) \text{ and } y \in \mathit{partner}(f,x)\,]\} \ .$$

First of all we note that, by construction, $\mathcal{A}$ is a resource-minimal reaction system. We will demonstrate now that (ζ) holds for $\mathcal{A}$, meaning that (since $\mathcal{A}$ is resource-minimal) $\mathit{res}_{\mathcal{A}} = f$.

Claim 10. $f \subseteq \mathit{res}_{\mathcal{A}}$, *i.e.*, $(\forall T \subseteq S)\ [\,f(T) \subseteq \mathit{res}_{\mathcal{A}}(T)\,]$.

Proof (Claim 10). Let $T \subseteq S$. We consider two cases.

Case 1: T is such that $f(T) = \varnothing$. Then, trivially, $f(T) \subseteq res_{\mathcal{A}}(T)$.

Case 2: T is such that $f(T) = \{q\}$. Then, by Claim 8, $(\exists x \in T)\,[\,x \in special\,(f,T))\,]$ and, by Claim 9, $(\exists y \notin T)\,[\,y \in partner(f,x)\,]$. Hence A contains a reaction $b = (\{x\},\{y\},\{q\})$. Clearly, b is enabled at T and, consequently, $q \in res_{\mathcal{A}}(T)$. Hence $f(T) = \{q\} \subseteq res_{\mathcal{A}}(T) = \{q\}$.

Thus the claim holds. *(Claim 10)* □

Claim 11. *$res_{\mathcal{A}} \subseteq f$, i.e., $(\forall T \subseteq S)\,[\,res_{\mathcal{A}}(T) \subseteq f(T)\,]$.*

Proof (Claim 11). Let $T \subseteq S$. We consider two cases.

Case 1: $res_{\mathcal{A}}(T) = \varnothing$. Then, trivially, $res_{\mathcal{A}}(T) \subseteq f(T)$.

Case 2: $res_{\mathcal{A}}(T) = \{q\}$. Then $(\exists a \in A)\,[\,en_T(a)\,]$. Therefore $a = (\{x\},\{y\},\{q\})$ where $x \in T$, $y \notin T$ and $y \in partner(f,x)$. Consequently, $f(T) = \{q\}$, and so $res_{\mathcal{A}}(T) = \{q\} \subseteq f(T) = \{q\}$.

Thus the claim holds. *(Claim 11)* □

From Claims 10 and 11 we get $res_{\mathcal{A}} = f$, and since $res_{\mathcal{A}}$ is a resource-minimal reaction system, (ζ) holds. Thus the assumption that (η) holds implies that (ζ) holds. This concludes the proof of Part 2. *(Part 2)* □

The proposition now follows from Part 1 and Part 2. *(Theorem 3)* □

8 Resource-Minimal rs Functions

In this section we generalise Theorem 3 to arbitrary rs functions.

We begin by decomposing reaction systems into a set of "specialised entity" reaction systems, where each such component rs is dedicated to producing one specific entity.

For a given reaction system $\mathcal{A} = (S, A)$ and $q \in S$, we define a reaction system $\mathcal{A}^q = (S, A^q)$, where:

$$A^q = \{(R_a, I_a, \{q\}) : a \in A \text{ and } q \in P_a\}\ .$$

Indeed, the set of specialised entity reaction systems $\mathcal{A}^q$ is equivalent to the original rs $\mathcal{A}$, as stated by the following result. Below $\bigcup_{q\in S} \mathcal{A}^q$ denotes the rs which is the union of the reaction systems $\mathcal{A}^q$, i.e., the rs $(S, \bigcup_{q\in S} \mathcal{A}^q)$.

Theorem 4 (Normal Form). *Let $\mathcal{A} = (S, A)$ be a reaction system.*

(i) $\mathcal{A} \sim \bigcup_{q\in S} \mathcal{A}^q$.

(ii) *$\mathcal{A}$ is resource-minimal iff each A^q is resource-minimal.*

Proof. (i) Let $\mathcal{A}' = \bigcup_{q \in S} \mathcal{A}^q$. Let $a_q = (R_a, I_a, \{q\})$, for all $q \in S$ and $a \in A$ satisfying $q \in P_a$. Clearly,

$$(\forall T \subseteq S)(\forall a \in A)\ [\, res_a(T) = \bigcup_{q \in P_a} res_{a_q}(T)\,]\ .$$

Hence

$$(\forall T \subseteq S)\ [\, \bigcup_{a \in A} res_a(T) = \bigcup_{a \in A} \bigcup_{q \in P_a} res_{a_q}(T)\,]\ ,$$

which yields

$$(\forall T \subseteq S)\ [\, res_{\mathcal{A}}(T) = res_{\mathcal{A}'}(T)\,]\ .$$

Thus $\mathcal{A} \sim \bigcup_{q \in S} \mathcal{A}^q$.

(ii) Follows immediately from the definitions. □

The decomposition of reaction systems into specialised entity reaction systems translates into specialised entity rs functions as follows.

Given an rs function $f : 2^S \to 2^S$ and $q \in S$, $f^q : 2^S \to 2^S$, the *specialised entity q-component of* f, is defined by:

$$(\forall T \subseteq S)\ [\, f^q(T) = f(T) \cap \{q\}\,]\ .$$

Observe that $(\forall T \subseteq S)\ [\, f(T) = \bigcup_{q \in S} f^q(T)\,]$.

Our basic notions of union-subadditivity and intersection-subadditivity can be transferred back and forth between rs functions and their specialised entity components as follows.

Theorem 5 (Distributivity). *Let f be an rs function.*

(i) f is union-subadditive iff each f^q is union-subadditive.

(ii) f is intersection-subadditive iff each f^q is intersection-subadditive.

Proof. (i) Let f be union-subadditive and $q \in S$. Then,

$$(\forall X, Y \subseteq S)\ [\, f(X \cup Y) \subseteq f(X) \cup f(Y)\,]\ .$$

Hence

$$(\forall X, Y \subseteq S)\ [\, f(X \cup Y) \cap \{q\} \subseteq (f(X) \cap \{q\}) \cup (f(Y) \cap \{q\})\,]\ .$$

Thus, by definition of f^q,

$$(\forall X, Y \subseteq S)\ [\, f^q(X \cup Y) \subseteq f^q(X) \cup f^q(Y)\,]\ .$$

As a result f^q is union-subadditive.

Suppose now that each f^q is union-subadditive. This means that

$$(\forall X, Y \subseteq S)(\forall q \in S)\ [\, f^q(X \cup Y) \subseteq f^q(X) \cup f^q(Y)\,]\ ,$$

which gives

$$(\forall X, Y \subseteq S)\ [\bigcup_{q\in S} f^q(X \cup Y) \subseteq \bigcup_{q\in S} f^q(X) \cup \bigcup_{q\in S} f^q(Y)]\ .$$

Since

$$(\forall X \subseteq S)\ [\, f(X) = \bigcup_{q\in S} f^q(X)\,]\ ,$$

we obtain

$$(\forall X, Y \subseteq S)\ [\, f(X \cup Y) \subseteq f(X) \cup f(Y)\,]\ .$$

As a result, f is union-subadditive.

(ii) Similar to the proof of (i). □

We are now ready to prove the main result of this section.

Theorem 6. *Let, for a finite nonempty set S, $f : 2^S \to 2^S$ be an rs function. Then the following statements are equivalent:*

- (θ) *f is resource-minimal.*
- (κ) *f is both union- and intersection-subadditive.*

Proof. As for Theorem 3, the proof is broken down into two parts.

Part 1. $(\theta) \implies (\kappa)$.

Proof (Part 1). Assume (θ), i.e., there exists a resource-minimal reaction system $res_{\mathcal{A}} = (S, A)$ which implements f, hence $res_{\mathcal{A}} = f$. By Theorem 4,

$$res_{\mathcal{A}} = \bigcup_{q\in S} res_{\mathcal{A}^q}\ .$$

Thus $f = \bigcup_{q\in S} f^q$. Since each f^q is a focus rs function, by Theorem 3:

$$(\forall q \in S)\ [\, f^q \text{ is union- and intersection-subadditive}\,]\ .$$

Hence by Theorem 5, function f is union- and intersection-subadditive. Therefore (κ) holds.

This concludes the proof of the first part. *(Part 1)* □

Part 2. $(\kappa) \implies (\theta)$.

Proof (Part 2). Assume (κ), i.e., f is union- and intersection-subadditive. As stated before Theorem 5, $f = \bigcup_{q\in S} f^q$, and by Theorem 5 each f^q is union- and intersection-subadditive. Since, obviously, each f^q is a focus function, by Theorem 3, each f^q satisfies (θ), i.e.,

$$(\forall q \in S)(\exists \mathcal{A}^q)\ [\, \mathcal{A}^q \text{ is a resource-minimal rs such that } res_{\mathcal{A}^q} = f^q\,]\ .$$

Obviously,

$$\bigcup_{q\in S} res_{\mathcal{A}^q} = \bigcup_{q\in S} f^q = f\ .$$

Let now $\mathcal{A}$ be the union of all $\mathcal{A}^q$, i.e., $\mathcal{A} = \bigcup_{q\in S} \mathcal{A}^q = (S, \bigcup_{q\in S} A^q)$. Since each $\mathcal{A}^q$ is resource-minimal, so is $\mathcal{A}$. Clearly:

$$\bigcup_{q\in S} res_{\mathcal{A}^q} = res_{\mathcal{A}} \ , \text{ and so } \bigcup_{q\in S} f^q = f = res_{\mathcal{A}} \ .$$

Clearly $\mathcal{A}$ is a resource-minimal reaction system, and so (θ) holds. This concludes the proof of Part 2. *(Part 2)* □

The theorem follows now from Part 1 and Part 2. □

9 Discussion

Given a reaction system $\mathcal{A} = (S, A)$ its result function $res_{\mathcal{A}}$ is determined/programmed by its set of reactions A. Hence, one of the fundamental questions is: what are the result functions that can be programmed by reactions systems with minimal resources? The goal of this paper is to provide an answer to this question, i.e., to provide characterisations of reactant-minimal, inhibitor-minimal, and resource-minimal rs functions. This goal was achieved and the corresponding characterisations are given by Theorems 1, 2 and 6, respectively.

These results can be used to expand the understanding of rs functions. Here are two examples of such usage.

(1) It is not obvious that knowing that an rs function can be implemented by a reaction-minimal rs *and* that it can also be implemented by an inhibitor-minimal rs implies that it can be implemented by an rs which is *both* reaction-minimal and inhibitor-minimal (i.e., an rs which is resource-minimal). However using our characterisation theorems, we can prove that this is the case.

Corollary 1. *An rs function is resource-minimal iff it is both reactant-minimal and inhibitor-minimal.*

Proof. Directly from Theorem 1, Theorem 2 and Theorem 6. □

(2) It was proved in [10] that increasing the number of resources leads to a strict hierarchy, i.e., for a given background set S with $|S| = s$, increasing the number of resources (allowed in the reactions of reaction systems with background S) from 2 up to s yields a strict hierarchy of classes of functions implementable by so restricted functions. Resource-minimal rs functions is the lowest class in this hierarchy.

The question arises whether restricting the number of reactants which can be used in any reaction to only one (or dually the number of inhibitors that can be used in any reaction to only one) is a real restriction. In other words, perhaps each rs function is implementable by an rs where each reaction uses only one reactant with no limitation on the number of inhibitors used (or dually each reaction uses only one inhibitor, with no limitation on the number of reactants used).

Using the characterisation results from this paper, we provide a negative answer to these two questions.

First we demonstrate in an elementary way that inhibitor-minimal reaction systems are not "universal" for the class of all rs functions.

To this aim consider reaction system $\mathcal{A} = (S, A)$ with

$$S = \{1, 2, 3\} \text{ and } A = \{(\{1\}, \{2, 3\}, \{1\})\} .$$

Obviously $\mathcal{A}$ is a (reactant-minimal) reaction system implementing the rs function:

$$f : 2^S \to 2^S \text{ with } f(X) = \begin{cases} \{1\} & \text{if } X = \{1\} \\ \varnothing & \text{otherwise} . \end{cases}$$

Consider now $\mathcal{F} = \{\{1, 2\}, \{1, 3\}\}$. Then:

$$f\big(\bigcap \mathcal{F}\big) = f(\{1\}) = \{1\} , \text{ while } f(\{1, 2\}) \cup f(\{1, 3\}) = \varnothing \cup \varnothing = \varnothing .$$

Hence $f\big(\bigcap \mathcal{F}\big) \not\subseteq \bigcup f(\mathcal{F})$, and so f is not intersection-subadditive. Consequently, by Theorem 2, f cannot be implemented by an inhibitor-minimal reaction system.

Note that $\mathcal{A}$ is reactant-minimal. Hence, there are even reactant-minimal rs functions which are not implementable by reaction systems with minimal inhibitor sets.

Now, we demonstrate that reactant-minimal reaction systems are also not universal for the class of all rs functions.

To this aim consider reaction system $\mathcal{A} = (S, A)$ with

$$S = \{1, 2, 3\} \text{ and } A = \{(\{1, 2\}, \{3\}, \{1\})\} .$$

Obviously $\mathcal{A}$ is a (inhibitor-minimal) reaction system implementing the rs function:

$$f : 2^S \to 2^S \text{ with } f(X) = \begin{cases} \{1\} & \text{if } X = \{1, 2\} \\ \varnothing & \text{otherwise} . \end{cases}$$

Consider now $\mathcal{F} = \{\{1\}, \{2\}\}$. Then:

$$f(\bigcup \mathcal{F}) = f(\{1, 2\}) = \{1\} , \text{ while } f(\{1\}) \cup f(\{2\}) = \varnothing \cup \varnothing = \varnothing .$$

Hence $f(\bigcup \mathcal{F}) \not\subseteq \bigcup f(\mathcal{F})$, and so f is not union-subadditive. Consequently, by Theorem 1, f cannot be implemented by a reactant-minimal reaction system.

Note that $\mathcal{A}$ is inhibitor-minimal. Hence, there are even inhibitor-minimal rs functions which are not implementable by reaction systems with minimal reactant sets.

The situation is quite different when one considers product-minimal reaction systems (i.e., reaction systems where for each reaction its product set is a singleton). One can then prove (see [5]) that for each rs function f there exists a product-minimal reaction system implementing f. Hence product-minimal reaction systems are universal.

A natural research topic (and perhaps a quite challenging open problem) to follow up the research presented in this paper is a characterisation of rs functions implementable by reaction systems using reactions with the number of reactants or/and inhibitors limited by k reactants, or k inhibitors, or k resources (with $k \geq 2$ for the number of reactants or the number of inhibitors, and $k \geq 3$ for the number of resources).

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