



Immersing reaction system specifications in evaluating environments

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Abstract

We propose an extension to the framework of reaction systems such that the environment not only plays the role of contributing entities to the successor state, but also influences the actual generation of products. In particular, we consider that an environment can assign *valences* to entities, be they used as reactants or inhibitors in a reaction, as well as *select* the entities which can appear in the successor state as product of a reaction. This provides a framework for *immersing* reaction system specifications into different contexts. We also derive a notion of *polarised reaction systems*, where entities can appear only as reactants or inhibitors in any given reaction. We compare the expressive power of the models, also showing some equivalences between them, and test them on three case studies derived from physiology, ecology, and chemistry.

Keywords Reaction systems · Valence · Polarity · Environmental influence

1 Introduction

Reaction systems constitute a nature-inspired model of computation (Ehrenfeucht and Rozenberg 2007), where system evolution is defined by combining the effects of internal transition rules, called *reactions*, with contributions from the environment. In this model, a *state* is a set of *entities*

taken from a *background set* S , and a reaction is defined by a triple composed of three subsets of S : R , the set of *reactants*, required *to be present* in the current state; I , the set of *inhibitors*, required *not to be present* in the current state; and P , the set of *products*, to be inserted into the successor state. Hence, a reaction $\rho = (R, I, P)$ is *enabled* in any state $W \subseteq S$ if and only if $R \subseteq W$, $I \cap W = \emptyset$. Note that ρ can be enabled in a state W only if $R \cap I = \emptyset$. The effect of the simultaneous application of all enabled reactions from a set A in W (noted $\text{res}_A(W)$), is given by the set-theoretic union of all of their P components. The construction of the successor state of W is then completed by set-theoretic union with a *context* provided by the environment.

This paper is situated in a line of research aimed at structuring the environment and extending its role (see Bottoni et al. 2019, 2020). In particular, we observe that an environment can influence the actual enabling and application of reactions through two types of actions. First, we consider that an environment can affect the relevance of an entity in a reaction, and model this phenomenon by equipping an environment with an *evaluator function*, assigning *valences* to the entities in the reactants and inhibitors (collectively known as *resources*) of reactions: only those reactions can be applied for which the total valence of reactants is greater than that of inhibitors. Hence, a triple (R, I, P) does not completely specify the conditions for its applicability, as in the classical model, since it can meet favourable or unfavourable conditions in a given state and environment.

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This notion stems from the observation that entities can appear to be inactive or with limited activity when immersed in different environmental conditions, for example under extreme temperatures, whether in the cold or in the heat, or under various levels of pollution. Conversely, their activity can be amplified under the same or other conditions, e.g., in phase-transition situations or under intense lighting. While such conditions can be qualitatively represented by suitable entities used as reactants or inhibitors, their being put on a par with entities representing actual elements may lead to less intuitive models, as will be shown in the examples of Section 6.

Our proposed second extension, aligning with a general view of the roles of entities (see e.g., Bottoni et al. 2002; Ehrenfeucht and Rozenberg 2003; Genova and Jonoska 2012), stems by recognising that a given entity may act either as a facilitator or as an inhibitor depending on environmental conditions; we model this case by letting the valuation function assign positive or negative valences to entities. In this new model, instead of immersing a reaction system into an environment, the latter is presented with what we call a *resource-product specification*, formed by two sets of entities. The first set lists entities which will receive their role from the environment: positively valued entities play the role of reactants and negatively valued ones that of inhibitors. Then, the enabling of the *resource* component of the specification depends on the comparison of their total weights as in the previous case. Moreover, since the execution of the specification may result in different effects, depending on the environment, the *product* component presents candidate products, from which the environment *selects* those entities which are actually produced under the current conditions.

When the set of valences is restricted to $\{-1, 1\}$, we say that entities are *polarised*, and enabling depends on comparing the respective cardinalities of positively and negatively polarised entities in the current state.

For all these models, we distinguish between *strong* and *weak* forms of enabling. While weak enabling is only based on the comparison of the respective total weights, strong enabling requires, in addition, the satisfaction of the classical condition that the set of reactants be fully contained in the current state. In both cases, the classical condition that no inhibitor be contained in the current state is waived. Consequently, the classical property $\text{res}_A(S) = \emptyset$ does not necessarily hold, so that the introduction of valences leads to the definition of a new class of behaviours.

Finally, we observe that a polarising environment induces a partitioning of S between positively valued entities and negatively valued ones. Hence, we explore the family of *polarised reaction systems*, in which a subset of entities can appear only as reactants and its complement with respect to

the background set only as inhibitors in all the reactions of the system. Interestingly, we prove that such systems can simulate the behaviour of unrestricted reaction systems.

We provide a formal account of these models and discuss their behaviours.

The contribution of the paper is therefore twofold. From the theoretical point of view we introduce the new notions of *evaluating environment* and of *resource-product specification* and the relative predicates for enabling and executing specifications, showing that they allow the expression of new types of behaviour. From the modelling point of view, we show that the notion of environment supports a flexible form of modelling, where the same collection of resources can be activated in different ways, producing different results, when immersed in different environments.

Paper structure. Section 2 recalls fundamental notions about reaction systems, presents the definition of process adopted in the paper, and introduces the notions of valence function and of evaluating environment, also providing a quick reference to the notation used in the paper. Then, Section 3 considers the dynamics resulting from the immersion of a reaction system into an environment assigning valences to reactants and environments, while Section 4 introduces resource-product specifications and the effect of their immersion into evaluating environments. For both of these models, the resulting dynamics are compared to those of classical reaction systems, showing that all versions of evaluating environments define new types of interactive process. Considerations on reactions derived from immersion into polarising environments as well as on polarised reaction systems are given in Section 5. After that, Section 6 illustrates some examples of immersion into evaluating environments to model systems from the biomedical, ecological, and chemical domains. Finally, Section 7 discusses related work and Section 8 draws conclusions and points to future work.

2 Background and preliminaries

We present notational conventions and basic notions on reaction systems, before introducing the new notions of valence and evaluating environment. For a quick reference to the most relevant notation used throughout the paper, Table 1 illustrates the names of the various families of entities and processes referred to in the paper, while Table 2 recalls the various definitions of enabling characterising the derived behaviours. In both cases, the last column points to the relevant definition in the paper.

Table 1 A table summarising the notation for the families of specifications in the paper

Notation	Meaning	Def.
(CI)PROC($\mathcal{A}$)	Set of (context-independent) processes in $\mathcal{A}$	3
VAL(S)	Set of valence functions over $S (v : S \rightarrow \mathbb{Z})$	4
PEV(S)	Set of positively evaluating environments over $S (val : S \rightarrow \mathbb{N})$	7
(CI)PROC $_t$ ($\mathcal{A}, pev$)	Set of (context-independent) processes, of type $t \in \{\text{strong}, \text{weak}\}$, in $\mathcal{A}$ under the positive environment pev	7
RP(S)	Set of resource-product specifications over $S ((X, Y) \in \wp(S) \times \wp(S))$	8
REV(S)	Set of relativising environments over $S (val : S \rightarrow \mathbb{Z}, sel : S \rightarrow \{0, 1\})$	11
(CI)PROC $_t$ (RP, rev)	Set of (context-independent) processes, of type $t \in \{\text{strong}, \text{weak}\}$, generated by immersing the set RP of resource-product specifications into the relativising environment rev	11
PLV(S) $\subseteq$ REV(S)	Set of polarising environments over $S (val : S \rightarrow \{-1, 1\}, sel : S \rightarrow \{0, 1\})$	13
(CI)PROC $_t$ (RP, plv)	Set of (context-independent) processes, of type $t \in \{\text{strong}, \text{weak}\}$, generated by immersing the set RP of resource-product specifications into the polarising environment plv	13
PRS(S)	Set of polarised reaction systems over S	16

2.1 Notation

As usual, $\mathbb{Z}$ is the set of integers, with $\mathbb{Z}^-, \mathbb{Z}^+$ respectively denoting negative and positive integers, so that $\mathbb{N} = \mathbb{Z} \setminus \mathbb{Z}^-$ is the set of natural numbers (including 0). For $n \in \mathbb{N}$, the interval $[1, n]$, of positive integers up to n is denoted by $\bar{n}$. Accordingly, $\bar{0}$ corresponds to the empty set. For $x \in \mathbb{Z}$, we denote by $abs(x)$ its absolute value, i.e., $max(x, -x)$. For a finite¹ set X , we denote its *cardinality* by $card(X)$ and its *powerset* by $\wp(X)$. In general, we rely on standard notions from set theory. With $f : X \rightarrow Y$ a function, we call X the domain of f (noted $dom(f)$), Y the *codomain* of f (noted $cod(f)$) and $\{y \in Y \mid \exists x \in X [y = f(x)]\}$ the *image* of f (noted $img(f)$). The notation $f : X \twoheadrightarrow Y$ (resp., $f : X \leftrightarrow Y$) indicates that f is *surjective* (resp., *bijective*). With $U \in \wp(X)$, the notation $f(U)$ stands for $\{f(x) \mid x \in U\}$. Analogously, for a *sequence* $\tau = \langle x_1, \dots, x_n \rangle \in X^n$, we denote by $f(\tau)$ the sequence $\langle f(x_1), \dots, f(x_n) \rangle \in Y^n$.

2.2 Reaction systems

We revise standard notions for reaction systems, relying on Ehrenfeucht and Rozenberg (2007) for the classical setting and on a view of processes developed in Bottoni et al. (2025).

Definition 1 (Background set and configuration). A finite set S with $card(S) \geq 2$ is called a *background set* and the set of all background sets is denoted by $\mathcal{S}$. With $S \in \mathcal{S}$, let $D, C, W \in \wp(S)$ be such that $W = D \cup C$. Then, $\kappa = (D, C, W)$ is called a *configuration over S* . We denote the set of configurations over S by $\mathcal{K}(S)$.

In the rest of the paper, the notation W^c stands for $S \setminus W$, for $W \in \wp(S)$.

Definition 2 (Reaction system). With $S \in \mathcal{S}$, a *reaction over S* is a triple $\rho = (R_\rho, I_\rho, P_\rho) \in (\wp(S) \setminus \emptyset)^3$ such that $R_\rho \cap I_\rho = \emptyset$. A *reaction system over S* (also noted *rs*) is then a pair $(S, \mathcal{A})$ for some set of reactions $\mathcal{A}$ over S . We denote by $R(S), RS(S)$ the sets of reactions and reaction systems over S , respectively.

Given $\rho \in R(S)$, the set $R_\rho \cup I_\rho$ is called the set of *resources* of ρ and is denoted by M_ρ , while the set $M_\rho \cup P_\rho$ is denoted by S_ρ and called the *background set* of ρ . Analogously, given $A \in \wp(R(S))$, we denote by $R(A), I(A), P(A), M(A)$, the sets $\bigcup_{\rho \in A} R_\rho, \bigcup_{\rho \in A} I_\rho, \bigcup_{\rho \in A} P_\rho, R(A) \cup I(A)$, respectively. From here on, for components of a reaction which are singletons, we represent $\{x\}$ simply with x .

¹ We only deal here with finite background sets, in accordance with the classical theory of reaction systems.

Table 2 A table summarising the enabling predicates for the dynamics presented in the paper

Notation	Alt. notation	Textual reading	Formal expression	Def.
$\rho \in R(S)$	$\rho = (R, I, P)$	Reaction over S	$R, I, P \in \wp(S) \setminus \emptyset$	2
$\text{en}_\rho(W)$	$\rho \in \text{EN}(\mathcal{A}, W)$	ρ enabled in $W \subseteq S$	$R \subseteq W, I \cap W = \emptyset$	3
$\text{wen}_\rho^{pev}(W)$	$\rho \in \text{WEN}(W, pev)$	ρ weakly enabled in $W \subseteq \text{Sunder } pev$	$\sum_{x \in R \cap W} val(x) > \sum_{x \in I \cap W} val(x)$	7
$\text{sen}_\rho^{pev}(W)$	$\rho \in \text{SEN}(W, pev)$	ρ strongly enabled in $W \subseteq \text{Sunder } pev$	$\rho \in \text{WEN}(\mathcal{A}, W) \wedge R \subseteq W$	7
$\text{wen}_{rp}^{rev}(W)$		rp weakly enabled in $W \subseteq \text{Sunder } rev$	$\sum_{x \in X \cap W} val(x) > 0$	11
$\text{sen}_{rp}^{rev}(W)$		rp strongly enabled in $W \subseteq \text{Sunder } rev$	$\text{sen}_{rp}^{rev}(W) \wedge R \subseteq W$	11
$\text{wen}_{rp}^{plv}(W)$		rp weakly enabled in $W \subseteq \text{Sunder } plv$	$\text{card}(X^+ \cap W) > \text{card}(X^- \cap W)$	13
$\text{sen}_{rp}^{plv}(W)$		rp strongly enabled in $W \subseteq \text{Sunder } plv$	$\text{wen}_{rp}^{plv}(W) \wedge R \subseteq W$	13

Definition 3 (Dynamics of reaction systems). Let $S \in \mathcal{S}$. Then,

- Let $W \in \wp(S)$. Then, we define the following:
 - With $\rho = (R, I, P) \in R(S)$, we say that ρ is *enabled* in W , noted $\text{en}_\rho(W)$, if $R \subseteq W, I \cap W = \emptyset$.
 - The *result* of the *application* of ρ in W , noted $\text{res}_\rho(W)$, is given by: $\text{res}_\rho(W) = P$ if $\text{en}_\rho(W)$ holds; $\text{res}_\rho(W) = \emptyset$ otherwise.
- Let $\mathcal{A} \in \wp(R(S)), \mathcal{A} = (S, A) \in \text{RS}(S)$. Then, we define the following:
 - The *enabled set* of A in W , $\{\rho \in A \mid \text{en}_\rho(W)\}$, is denoted by $\text{EN}(A, W)$.
 - The *application* of A (resp., $\mathcal{A}$) in W , noted $\text{res}_A(W)$ (resp., $\text{res}_{\mathcal{A}}(W)$), is given by $\bigcup \{\text{res}_\rho(W) \mid \rho \in A\} = \bigcup \{P_\rho \mid \rho \in \text{EN}(A, W)\}$.
 - Let $\kappa = (D, C, W), \kappa' = (D', C', W') \in \mathcal{K}(S)$ be such that $D' = \text{res}_{\mathcal{A}}(W)$. Then we say that (κ, κ') is a *(interactive) process step* in $\mathcal{A}$.
 - A *(interactive) process* in $\mathcal{A}$ is a sequence $\pi = \langle (\kappa_0, \kappa_1), \dots, (\kappa_{n-1}, \kappa_n) \rangle$ of process steps in $\mathcal{A}$. Then, $n \geq 1$ is the *length* of π , noted $|\pi|$. For a process π in $\mathcal{A}$, we call $\kappa_\pi = \langle \kappa_0, \dots, \kappa_n \rangle$ its *configuration sequence*.

With π a process and $i \in \overline{|\pi|}$, we denote by $\kappa_\pi[i]$ the configuration *reached* by π at step i , and by $\kappa_\pi[0]$ its *initial configuration*. For the following sequences derivable from κ_π , we use the same indexing convention. Indeed, given $\kappa_\pi = \langle (D_0, C_0, W_0), \dots, (D_n, C_n, W_n) \rangle$, we recover the usual notions of *result*, *context*, and *state sequence* of π , as $\delta_\pi = \langle D_0, \dots, D_n \rangle, \gamma_\pi = \langle C_0, \dots, C_n \rangle, \sigma_\pi = \langle W_0, \dots, W_n \rangle$, respectively². A process π is *context-independent* if, for $i \in \overline{|\pi|}$, we have $C_i \subseteq D_i$. We do not require $C_0 \subseteq D_0$ for context-independence, but we have $\sigma_\pi[i] = \delta_\pi[i]$ for $i \in \overline{|\pi|}$. Finally, the *enabled set sequence*, η_π is given by $\eta_\pi[i] = \text{EN}(A, W_i)$, for $i \in \{0, 1, \dots, n\}$.

With $\mathcal{A} \in \text{RS}(S)$, the set of its processes is denoted by $\text{PROC}(\mathcal{A})$ and the set of its context-independent processes is denoted by $\text{CIPROC}(\mathcal{A})$. For $\pi \in \text{CIPROC}(\mathcal{A})$, we also use the notation $\pi \in \text{CIPROC}_0(\mathcal{A})$ if $C_0 \subseteq D_0$.

Remark 1 For any process step (κ, κ') with $\kappa = (D, C, W), \kappa' = (D', C', W')$, we have $W \in \{\emptyset, S\} \implies D' = \emptyset$. Hence, in a context-independent

² The original definition has $D_0 = \emptyset, W_0 = C_0$, which is not required here.

process step we have $W \in \{\emptyset, S\} \implies W' = \emptyset$, and $W_i \in \{\emptyset, S\} \implies W_j = \emptyset$ for $j \in \{i+1, \dots, |\pi|\}$.

It is well known that for any function $f : \wp(S) \rightarrow \wp(S)$ satisfying the *boundary condition* $f(S) = f(\emptyset) = \emptyset$ there exists a reaction system $\mathcal{A}$ such that $\text{res}_{\mathcal{A}}(W) = f(W)$. In particular, one can always create the *maximally inhibited* reaction system defined by $A = \{(W, S \setminus W, f(W)) \mid f(W) \neq \emptyset\}$ (Salomaa 2012).

2.3 Valences and evaluating environments

The rest of the paper relies on the notions of *valence* function and *evaluating environment*, for which we refer to Definition 4.

Definition 4 (Valence function and evaluating environment). Let $S \in \mathcal{S}$. Then we define the following:

- A *valence function* over S is a function $f : S \rightarrow \mathbb{Z}$, such that $\text{cod}(f) \cap \mathbb{Z}^+ \neq \emptyset$. With $f(x) = k$, we also say that k is the *weight* of x . The set of valence functions over S is denoted by $\text{VAL}(S)$.
- An *evaluating environment* over S is defined by a set of valence functions $\emptyset \neq \mathcal{V} \in \wp(\text{VAL}(S))$, and is referred to as a pair $ev = (S, \mathcal{V})$. The set of evaluating environments over S is denoted by $\text{EV}(S)$.

In the following, for $W \subseteq S, f \in \text{VAL}(S)$, the notations W_f^-, W_f^0, W_f^+ (or simply W^-, W^0, W^+ when f is understood in the context of the situation) will stand for $\{x \in W \mid f(x) < 0\}, \{x \in W \mid f(x) = 0\}, \{x \in W \mid f(x) > 0\}$, respectively. Note that we admit $f(x) = 0$ for some $x \in S$, in which case we say that x is *inert* in ev . However, the case $\{x \in S \mid f(x) = 0\} = S$ is excluded, since by definition we have $S_f^+ \neq \emptyset$.

3 Immersing reactions into evaluating environments

We first study the case where $\mathcal{V}$ is a singleton containing a function assigning weights which are positive integers. When a standard reaction is *immersed* in an environment endowed with such a function, its applicability results from comparing the total weights for the sets of reactants and inhibitors. As shown in Section 6.1, this allows the modelling of phenomena requiring specific environmental conditions.

Definition 5 (Positively evaluating environment). Let $pev = (S, \{val\}) \in \text{EV}(S)$. If $\text{cod}(val) \subseteq \mathbb{N}$, then pev is a

positively evaluating environment (or *positive environment*, for short) over S and val is the *evaluator* for pev . The set of positive environments over S is denoted by $\text{PEV}(S)$.

While we admit $val(x) = 0$ for some $x \in Q \subsetneq S$, only entities with positive weight are considered in assessing whether a reaction is enabled. In particular, as it might be the case that a positive environment does not provide positive values for any of the resources found in a reaction, i.e., $R^+ = \emptyset$ or $I^+ = \emptyset$, Definition 6 establishes which reactions can be immersed in a given positive environment.

Definition 6 (Compatibility of reactions and positively evaluating environments). Let $\rho = (R, I, P) \in \text{R}(S_1)$, $pev = (S_2, \{val\}) \in \text{PEV}(S_2)$. Then, ρ is *positively compatible* with pev , noted $\text{comp}^+(\rho, pev)$, iff $M_\rho, S_\rho \subseteq S_2, R^+ \neq \emptyset \neq I^+$. With $A \in \wp(\text{R}(S_1))$, we have that $\text{comp}^+(A, pev)$ holds iff $\text{comp}^+(\rho, pev)$ holds for $\rho \in A$.

In other words, we require val to assign a value to all of the entities mentioned in ρ , and in particular to assign a positive value to at least one entity in both of R, I .

Remark 2 In general, with $\rho = (R, I, P) \in \text{R}(S_1)$, $pev \in \text{PEV}(S_2)$, we would just need $R^+ \neq \emptyset \neq I^+, M_\rho \subseteq S_2$. However, consistently with the notion that P is *produced* in the environment, we adopt the stricter condition $S_\rho \subseteq S_2$.

Definition 7 (Dynamics of positively valued reactions). With: $\rho = (R, I, P) \in \text{R}(S_1); W \in \wp(S_1); pev = (S_2, \{val\}) \in \text{PEV}(S_2); \text{comp}^+(\rho, pev)$, we write $v_R(W)$ for $\sum_{x \in R \cap W} val(x)$ and $v_I(W)$ for $\sum_{y \in I \cap W} val(y)$. Then:

- if $v_R(W) > v_I(W)$ holds, then we say that ρ is *weakly enabled* in W under pev , noted $\text{wen}_\rho^{pev}(W)$ (or $\rho \in \text{WEN}(W, pev)$); and
- if both of $v_R(W) > v_I(W), R \subseteq W$ hold, then we say that ρ is *strongly enabled* in W under pev , noted $\text{sen}_\rho^{pev}(W)$ (or $\rho \in \text{SEN}(W, pev)$).

The *weak* (resp., *strong*) application of ρ in W under pev is then given by $\text{wres}_\rho^{pev}(W) = P$ (resp., $\text{sres}_\rho^{pev}(W) = P$) if $\rho \in \text{WEN}(W, pev)$ (resp., if $\rho \in \text{SEN}(W, pev)$), and $\text{wres}_\rho^{pev}(W) = \emptyset$ (resp., $\text{sres}_\rho^{pev}(W) = \emptyset$) otherwise. The notions of weak/strong process step and interactive process for $\mathcal{A} = (S, A)$ immersed in pev are analogous to Definition 3, when substituting $\text{wres}_A^{pev}, \text{sres}_A^{pev}$ for res_A .

If, for t one of *weak*, *strong*, an interactive process π consists only of steps of type t then we say that π is of type t . We

denote the set of such (possibly context-independent) processes by $(\text{CI})\text{PROC}_t(\mathcal{A}, \text{pev})$ and use $(\text{CI})\text{PROC}(\mathcal{A}, \text{pev})$ to include also processes in which steps of different types appear.

Remark 3 For $\rho \notin \text{WEN}(W, \text{pev})$ it is necessary that $v_R(W) \leq v_I(W)$, whereas for $\rho \notin \text{SEN}(W, \text{pev})$ it is sufficient that one of $v_R(W) \leq v_I(W)$, $R \not\subseteq W$ holds. Of course, strong enabling implies weak enabling, i.e., $\rho \in \text{SEN}(W, \text{pev}) \implies \rho \in \text{WEN}(W, \text{pev})$. Similar considerations will hold for the other definitions of enabling in Section 4.

Example 1 With $S = \{x, y, w, z\}$, consider the reaction $\rho = (\{x, y\}, \{w, z\}, P)$, for some $\emptyset \neq P \subseteq S$, and the evaluator $\text{val} : S \rightarrow \mathbb{N}$, with $\text{val}(x) = 2$, $\text{val}(y) = \text{val}(w) = \text{val}(z) = 1$. Then, for $W \in \wp(S)$, applying ρ in $\text{pev} = (S, \{\text{val}\})$ produces the following set of results, that we contrast with the results for classical enabling. In particular, we consider the following cases for W :

- $\emptyset, \{w\}, \{z\}, \{w, z\}, \{y, w\}, \{y, z\}$:
 $\text{res}_\rho(W) = \text{sres}_\rho^{\text{pev}}(W) = \text{wres}_\rho^{\text{pev}}(W) = \emptyset$.
- $\{x\}, \{y\}, \{x, w\}, \{x, z\}$:
 $\text{res}_\rho(W) = \text{sres}_\rho^{\text{pev}}(W) = \emptyset$, $\text{wres}_\rho^{\text{pev}}(W) = P$.
- $\{x, y\}$: $\text{res}_\rho(W) = \text{sres}_\rho^{\text{pev}}(W) = \text{wres}_\rho^{\text{pev}}(W) = P$.
- $\{x, y\} \cup Q, \emptyset \neq Q \subseteq \{w, z\}$:
 $\text{res}_\rho(W) = \emptyset$, $\text{sres}_\rho^{\text{pev}}(W) = \text{wres}_\rho^{\text{pev}}(W) = P$.

Note that, in Example 1, both of ρ, pev are defined over S . Since $S_\rho = S$, we could have val defined over any S_2 such that $S_2 \supseteq S$. For simplicity, here and henceforth, we take $S_1 = S_2 = S$, for some $S \in \mathcal{S}$.

Theorems 1 and 2 show that valences introduce a new type of dynamics. Indeed, ρ may not be “classically” enabled in W (due to the presence of inhibitors), yet be strongly (and hence weakly) enabled when immersed in a suitable positive evaluating environment. On the other hand, if ρ is classically enabled in W , it is strongly (and hence weakly) enabled in any positive environment.

Theorem 1 Let $\rho = (R_\rho, I_\rho, P_\rho) \in \mathcal{R}(S)$. Then, the following hold:

- There exist $\text{pev} = (S, \{\text{val}\}) \in \text{PEV}(S)$, $W \in \wp(S)$, with $\text{comp}^+(\rho, \text{pev})$, such that We follow an argument analogous to that in the proof $\text{res}_\rho(W) = \emptyset$, $\text{sres}_\rho^{\text{pev}}(W) = \text{wres}_\rho^{\text{pev}}(W) \neq \emptyset$.
- Let $\text{pev} = (S, \{\text{val}\}) \in \text{PEV}(S)$, $\text{comp}^+(\rho, \text{pev})$. Then, for any given $W \in \wp(S)$, we have $\text{en}_\rho(W) \implies \rho \in \text{SEN}(W, \text{pev})$ (hence, $\text{res}_\rho(W) = \text{sres}_\rho^{\text{pev}}(W) = P_\rho$).

Proof We prove the two items separately.

(ad I.) Let val be such that $\text{val}(x) = 2 \times \text{card}(I_\rho)$ for $x \in R_\rho$, and $\text{val}(x) = 1$ for $x \in I_\rho$. Then, with $W = R_\rho \cup I_\rho$, we have $v_R(W) = 2 \times \text{card}(I_\rho) \times \text{card}(R_\rho \cap W) = 2 \times \text{card}(R_\rho) \times \text{card}(I_\rho)$, $v_I(W) = \text{card}(I_\rho \cap W) = \text{card}(I_\rho)$. Since $R_\rho \subseteq W$ and neither intersection is empty, we have $v_R(W) > v_I(W)$, hence $\text{sres}_\rho^{\text{pev}}(W) = P_\rho$. Conversely, since $I_\rho \cap W \neq \emptyset$, we have $\text{res}_\rho(W) = \emptyset$.

(ad II.) Immediate from the fact that $\text{en}_\rho(W) \implies R_\rho \subseteq W, I_\rho \cap W = \emptyset$. Then, by definition of positive compatibility (Definition 6), we have $V_{R_\rho}(W) > 0 = V_I(W)$. $\square$

Theorem 2 There exist: $\mathcal{A} = (S, A), \text{pev} \in \text{PEV}(S)$ such that there exists $\pi \in \text{PROC}(\mathcal{A}, \text{pev})$ for which $\pi \notin \text{PROC}(\mathcal{A}')$ for any $\mathcal{A}' \in \mathcal{RS}(S)$.

Proof We follow an argument analogous to that in the proof of Item I. of Theorem 1. Let $A = \{\rho\}, \text{pev} = (S, \{\text{val}\})$ be such that $\rho = (S \setminus \{x\}, x, P)$ for some $x \in S, P \in \wp(S) \setminus \emptyset$, with $\text{val}(y) = 2$ for $y \neq x$, and $\text{val}(x) = 1$. Then, with $W = S$, we have $v_R(S) = 2 \times (\text{card}(S) - 1)$, $v_I(S) = 1$, so that $v_R(S) > v_I(S)$ by construction. Now, suppose that $\sigma_\pi[i] = S$; then we will have $\delta_\pi[i+1] = P \neq \emptyset$. On the other hand, for any choice of $D_i, C_i, C_{i+1}, D_i \cup C_i = S$, the process step $((D_i, C_i, S), (P, C_{i+1}, P \cup C_{i+1}))$ cannot appear in any process of any reaction system over S . The result holds for both strong and weak steps. $\square$

Observation 1 As $\text{wres}_A^{\text{pev}}, \text{sres}_A^{\text{pev}}$ need not satisfy the boundary condition (we still have $\text{wres}_A^{\text{pev}}(\emptyset) = \text{sres}_A^{\text{pev}}(\emptyset) = \emptyset$, but not necessarily $\text{wres}_A^{\text{pev}}(S) = \emptyset$, $\text{sres}_A^{\text{pev}}(S) = \emptyset$), we cannot directly construct an equivalent maximally inhibited reaction system over S . However, by working on a background set $S_\# = S \cup \{\#\}$, with $\# \notin S$, we construct the sets $B_A^w = \{(W, S_\# \setminus W, \text{wres}_A^{\text{pev}}(W)) \mid \text{wres}_A^{\text{pev}}(W) \neq \emptyset\}$, $B_A^s = \{(W, S_\# \setminus W, \text{sres}_A^{\text{pev}}(W)) \mid \text{sres}_A^{\text{pev}}(W) \neq \emptyset\} \in \wp(\mathcal{R}(S_\#))$, for which it is immediate to verify that $\text{res}_{B_A^w}(W) = \text{wres}_A^{\text{pev}}(W)$, $\text{res}_{B_A^s}(W) = \text{sres}_A^{\text{pev}}(W)$ for any $W \in \wp(S)$.

4 Immersing resource-product specifications into evaluating environments

We now consider evaluating environments in which to immerse not “classical” reactions defined as triples according to Definition 2, but a new type of specification, deemed here *resource-product specification* (see Definition 8). Such

specifications generalise the notions of *resource set* (M_ρ) and *product set* (P_ρ) of a reaction ρ by presenting two sets of entities that the environment will use to assign roles to resources and to determine the effect (the actual product) of the immersion.

Definition 8 (Resource-product specification). With $S \in \mathcal{S}$, a *resource-product specification over S* (shortly, *rp-spec*) is a pair $rp = (X, Y)$, for some $X, Y \in \wp(S) \setminus \emptyset, \text{card}(X) \geq 2$. The set of rp-specs over S is denoted by $\text{RP}(S)$.

The condition $\text{card}(X) \geq 2$ is requested to have enough entities to cover both positive and negative roles when immersed in an evaluating environment.

In Section 4.1 and Section 4.2 we will present evaluating environments characterised by two valence functions: an *evaluator*, through which it will assign positive (*reactant-like*) or negative (*inhibitor-like*) roles to the entities in X , and a *selector*, through which it will select from Y the entities apt to be produced.

4.1 Relativising environments

In the first model, we constrain the evaluator to also provide negative valences for some nonempty subset of S . In this case, we make explicit the role of the environment in assigning roles to resources in a resource-product specification as well as computing its effects by selecting from its candidate products (see Definition 8). As mentioned in Section 1, this reflects the fact that the immersion of entities in an environment can change the role the entities can play, as well as the global effect of the reactions.

A *relativising environment* (see Definition 9) is therefore equipped with two valence functions: the evaluator assigns weights, either positive or negative, to resources; and the selector establishes which of the candidate product entities will constitute the reaction products. New notions of compatibility (see Definition 10) and enabling (see Definition 11) ensue. In particular, depending on the sign assigned by the evaluator, entities will act as reactants or as inhibitors, with a strength depending on the assigned weight, and enabling will depend on the comparison of their respective weights.

Definition 9 (Relativising environment). Let $val, sel : S \rightarrow \mathbb{Z}$ be two valence functions, with $\text{cod}(sel) = \{0, 1\}$. If we have $\emptyset \neq S_{val}^-, S_{val}^+, S_{sel}^+$, then we say that $rev = (S, \{val, sel\}) \in \text{EV}(S)$ is a *relativising environment over S* . The set of relativising environments over S is denoted by $\text{REV}(S)$.

Functions val, sel are called, respectively, *evaluator* and *selector*. Then, based on the convention established in

Section 2.3, with $W \in \wp(S), f \in \{val, sel\}$, we write W_f^-, W_f^+ for $\{x \in W \mid f(x) < 0\}, \{x \in W \mid f(x) > 0\}$, respectively, and W_{sel}^0 for $\{x \in W \mid sel(x) = 0\}$. The notion of compatibility is now redefined in Definition 10 to take into account both of val, sel and is related to an *rp-spec* instead of a reaction.

Definition 10 (Compatibility of rp-specs and relativising environments). With $rp = (X, Y) \in \text{RP}(S)$, $rev = (S, \{val, sel\}) \in \text{REV}(S_2), X \cup Y \subseteq S_2$, let each of X^-, X^+, Y^+ be nonempty. Then, we say that rp and rev are *relatively compatible*, noted $\text{comp}_+^+(rp, rev)$.

Remark 4 The condition $\text{card}(X) \geq 2$ from Definition 8 is essential to allow both of X^-, X^+ to be nonempty, while a condition $Y^0 \neq \emptyset$ is not required.

Definition 11 (Relative dynamics). Let: $rp = (X, Y) \in \text{RP}(S_1); rev = (S_2, \{val, sel\}) \in \text{REV}(S_2); \text{comp}_+^+(rp, rev)$. We then define the function $v_X : \wp(S) \rightarrow \mathbb{Z}$, given, for $W \in \wp(S_2)$, by $v_X(W) = \sum_{x \in X \cap W} val(x)$. Now:

- if $v_X(W) > 0$ holds, then we say that rp is *weakly enabled in W under rev* (noted $\text{wen}_{rp}^{rev}(W)$); and
- if both of $v_X(W) > 0, X^+ \subseteq W$ hold, then we say that rp is *strongly enabled in W under rev* (noted $\text{sen}_{rp}^{rev}(W)$).

The *weak* (resp., *strong*) *execution of rp in W under rev* is then given by $\text{wres}_{rp}^{rev}(W) = P, \text{sres}_{rp}^{rev}(W) = P$ if $\text{wen}_{rp}^{rev}(W), \text{sen}_{rp}^{rev}(W)$ respectively hold, and $\text{sres}_{rp}^{rev}(W) = \text{wres}_{rp}^{rev}(W) = \emptyset$ otherwise.

The extension to $RP \in \wp(\text{RP}(S))$ of the notions of weak/strong process step and interactive process is immediate and analogous to Definition 7, when substituting $\text{wres}_{RP}^{rev}, \text{sres}_{RP}^{rev}$ for $\text{wres}_A^{pev}, \text{sres}_A^{pev}$.

Example 2 With $S = \{x, y, w, z\}$, let $rp = (\{x, y, w\}, \{w, z\}) \in \text{RP}(S), rev = (S, \{val, sel\}) \in \text{REV}(S)$, with $val(x) = 2, val(y) = val(w) = val(z) = -1$ and $sel(x) = sel(y) = sel(w) = 1, sel(z) = -1$. Then, for $W \in \wp(S)$, the execution of rp in $W \in \wp(S)$ under rev produces the following set of results.

- $W \in Q = \{\{x\}, \{x, y\}, \{x, w\}, \{x, z\}\} :$
 $\text{sres}_{rp}^{rev}(W) = \text{wres}_{rp}^{rev}(W) = \{w\}$
 $= \text{wres}_{rp}^{rev}(W) = \{w\}.$
- $W \in \wp(S) \setminus Q : \text{sres}_{rp}^{rev}(W) = \text{wres}_{rp}^{rev}(W) = \emptyset.$

It is to be noted that for no $\rho \in R(S)$ we could obtain $\rho(W) \neq \emptyset$ for all $W \in Q$, as it would amount to ρ not having any inhibitor in S .

If, for t one of *weak*, *strong*, an interactive process π consists only of steps of type t , then we say that π is of type t . We denote the set of such (possibly context-independent) processes generated by the immersion of a set RP of *rp-specs* into a relativising environment rev by $(CI)PROC_t(RP, rev)$ and use $(CI)PROC(RP, rev)$ to include also processes in which steps of different types appear.

The same considerations for the relation between weak and strong enabling for positive environments from Remark 3 hold for the versions in Definition 11.

Theorem 3 establishes a correspondence between dynamics in positive and relative environments, relying on the condition $X^- \neq \emptyset$.

Theorem 3 Let $\rho \in R(S), pev \in PEV(S), comp^+(\rho, pev)$. Then, there exist $rp \in RP(S), rev \in REV(S), comp^+(rp, rev)$, such that, for $W \in \wp(S)$, we have $wres_{rp}^{rev}(W) = wres_{\rho}^{pev}(W)$, $sres_{rp}^{rev}(W) = sres_{\rho}^{pev}(W)$.

Proof Suppose $\rho = (R, I, P), pev = (S, \{val_+\})$, for some evaluator val_+ . Then, we take $rev = (S, \{val_r, sel\})$ to be such that: (a) $val_+(x) = val_r(x)$ for $x \in X^+$ and $val_+(x) = -val_r(x)$ for $x \in X^-$; and (b) $R = X^+, I = X^-, P = Y^+$. $\square$

Theorem 4 Let $\rho \in R(S)$. Then, there exist $rp \in RP(S), rev = (S, \{val\}) \in REV(S), comp^+(rp, rev)$, such that, for $W \in \wp(S)$, we have $sres_{rp}^{rev}(W) = res_{\rho}(W)$.

Proof We define the functions val, sel as follows: $val(x) = 1$ if $x \in R_{\rho}, val(x) = -(|M_{\rho}| + 1)$ if $x \in I_{\rho}, val(x) = 0$ if $x \in S \setminus M_{\rho}$ and $sel(x) = 1$ if $x \in P_{\rho}, sel(x) = 0$ if $x \in S \setminus P_{\rho}$. $\square$

The equivalence between classical dynamics and relative dynamics for single reactions or valuations does not extend to whole reaction systems.

Theorem 5 There exists $A \in \wp(R(S))$ such that $res_A \neq sres_A^{rev}, wres_A^{rev}$ for any choice of $rp = (X, Y) \in \wp(RP(S)), rev \in REV(S), comp^+(rp, rev)$.

Proof It is sufficient to take any $A \supseteq \{a_1, a_2\}$, with $R_{a_1} \cap I_{a_2} \neq \emptyset$. $\square$

Conversely, Theorem 6 shows that the opposite direction yields an equivalence when taking the reaction system derived from the immersion in a relativising environment of a set of *rp-specs*.

Theorem 6 Let: $RP \in \wp(RP(S)), rev = (S, \{val_r, sel\}) \in REV(S)$ with $comp^+(RP, rev)$. Then, there exist: $(S, \{val_+\}) \in PEV(S)$ s.t., for $W \in \wp(S)$, we have $wres_{RP}^{rev}(W) = wres_A^{pev}(W), sres_{RP}^{rev}(W) = sres_A^{pev}(W)$.

Proof We take $A = \{(X^+, X^-, Y^+) | rp = (X, Y) \in RP\}$, with val_+ given by: $val_+ = val_r(x)$ for $x \in S^+$, and $val_+(x) = -val_r(x)$ for $x \in S^-$. $\square$

More significantly, Theorem 7 shows that the execution of *rp-specs* under relativising environments may give rise to behaviours different from those of any reaction system, generalising the observation made in Example 2 for a single reaction.

Theorem 7 There exist $RP \in RP(S), rev \in REV(S)$ such that there exists $\pi \in PROC(RP, rev)$ for which $\pi \notin PROC(A)$ for any $A \in RS(S)$.

Proof We follow an argument analogous to that in the proof of Theorem 2. Let $RP = \{S, (X, Y)\}, rev = (S, \{val, sel\})$ be such that $val(x) = 2$ for $x \in S_a$ and $val(x) = -1$ for $x \in S_b$, for some partition $\{S_a, S_b\}$ of S , with $card(S_b) = 1$. Then, with $W = S$, we have $v_R(S) = 2 \times card(S_a), v_I(S) = -1$, so that $v_R(S) > v_I(S)$ by construction. Now, suppose that $\sigma_{\pi}[i] = S$; then we have $\delta_{\pi}[i+1] = Y^+ \neq \emptyset$, but for any choice of $D_i, C_i, C_{i+1}, D_i \cup C_i = S$, the process step $((D_i, C_i, S), (Y^+, C_{i+1}, Y^+ \cup C_{i+1}))$ cannot appear in any process of any reaction system over S . The result holds for both strong and weak steps. $\square$

4.2 Polarising environments

A polarising environment is a special case of relativising environment, assigning to each entity a weight of either 1 or -1 , with the sign indicating their role as reactant or inhibitor. For simplicity, we refer to a single background set, S , and maintain the conventions for $X^-, X^+, Y^0, Y^+, W^-, W^+$.

Sections 6.2, 6.3 will show the relevance of this notion for modelling phenomena which can proceed in different ways under different environmental conditions.

Definition 12 (Polarising environment). Let $plv = (S, \{val, sel\}) \in REV(S)$. If $cod(val) = \{-1, 1\}$, then we say that plv is a *polarising environment* over S . The set of polarising environments over S is denoted by $PLV(S)$.

Definition 13 (Polarised dynamics). With: $rp = (X, Y) \in RP(S); plv = (S, \{val, sel\}) \in PLV(S); comp^+(rp, plv)$;

$W \in \wp(S); Q = X \cap W$, let $v_X(W) = \text{card}(Q^+) - \text{card}(Q^-)$. Then, consistently with Definition 11, we have:

- if $v_X(W) > 0$ holds, then we say that rp is *weakly enabled in W under plv* (noted $\text{wen}_{rp}^{plv}(W)$); and
- if both of $v_X(W) > 0, X^+ \subseteq W$ hold, then we say that rp is *strongly enabled in W under plv* (noted $\text{sen}_{rp}^{plv}(W)$).

The weak (resp., strong) execution of rp in W under plv is then given by $\text{wres}_{rp}^{plv}(W) = P, \text{sres}_{rp}^{plv}(W) = P$ if, respectively, $\text{wen}_{rp}^{plv}(W), \text{sen}_{rp}^{plv}(W)$ hold, and $\text{wres}_{rp}^{plv}(W) = \text{sres}_{rp}^{plv}(W) = \emptyset$ otherwise. The definitions of weak/strong process step and interactive process for rp immersed in plv result accordingly.

We use the notations $(\text{CI})\text{PROC}_t(RP, plv)$, for t one of strong, weak, and $(\text{CI})\text{PROC}(RP, plv)$ in accordance with those in Section 4.1.

Example 3 With $S = \{x, y, w, z\}$, let $rp = (\{x, y, w\}, \{w, z\}) \in \text{RP}(S)$, with $\text{val}(x) = \text{val}(y) = 1, \text{val}(w) = \text{val}(z) = -1, plv = (S, \{\text{val}, \text{sel}\}) \in \text{PLV}(S)$ and $\text{sel}(x) = \text{sel}(y) = \text{sel}(w) = 1, \text{sel}(z) = -1$. Then, for $W \in \wp(S)$, executing rp in W under plv produces the following set of results.

- $W \in Q_{wk} = \{\{x\}, \{y\}\} : \text{wres}_{rp}^{plv}(W) = \{w\}, \text{sres}_{rp}^{plv}(W) = \emptyset$
- $W \in Q_{sg} = \{\{x, y\}, \{x, y, w\}, \{x, y, z\}\} : \text{wres}_{rp}^{plv}(W) = \text{sres}_{rp}^{plv}(W) = \{w\}$
- $W \in \wp(S) \setminus (Q_{wk} \cup Q_{sg}) : \text{sres}_{rp}^{plv}(W) = \text{wres}_{rp}^{plv}(W) = \emptyset$.

It is to be noted that for no $\rho \in \text{R}(S)$ can we obtain $\text{res}_\rho(W) \neq \emptyset$ for all $W \in Q_{sg}$, as it would amount to ρ not having any inhibitor in S .

The same considerations as in Remark 3 hold for polarising environments. Theorem 8 establishes an equivalence between immersing a single rp -spec in a polarising environment and immersing a single reaction in a positive one.

Theorem 8 Let $rp = (X, Y) \in \text{RP}(S), plv = (S, \{\text{val}_r, \text{sel}\}) \in \text{PLV}(S), \text{comp}^+_{rp}(rp, plv)$. Then, there exist: $\rho \in \text{R}(S); \text{pev} = \rho \in \text{R}(S); \text{pev} = (S, \{\text{val}_+, \text{sel}\}) \in \text{PEV}(S); \text{comp}^+(\rho, \text{pev})$ such that $\text{sres}_{\rho}^{\text{pev}}(W) = \text{sres}_{rp}^{plv}(W), \text{wres}_{\rho}^{\text{pev}}(W) = \text{wres}_{rp}^{plv}(W)$ for any $W \in \wp(S)$. Conversely, for $\rho = (R, I, P) \in \text{R}(S); \text{pev} = (S, \{\text{val}_+, \text{sel}\}) \in \text{PEV}(S); \text{comp}^+(\rho, \text{pev})$, there exist: $rp = (X, Y) \in \text{RP}(S), plv = (S, \{\text{val}_r, \text{sel}\}) \in \text{PLV}(S), \text{comp}^+_{rp}(rp, plv)$ such that $\text{sres}_{\rho}^{\text{pev}}(W) = \text{sres}_{rp}^{plv}(W), \text{wres}_{\rho}^{\text{pev}}(W) = \text{wres}_{rp}^{plv}(W)$ for any $W \in \wp(S)$.

Proof For the first implication, we take $\rho = (X^+, X^-, Y^+)$, $\text{val}_+(x) = \text{abs}(\text{val}_r(x))$, for $x \in S$. For the second implication, we take $X = R \cup I, Y = P$, with $\text{val}_r(x) = 1$ if $x \in R, \text{val}_r(x) = -1$ otherwise; and $\text{sel}(x) = 1$ if $x \in Y, \text{sel}(x) = 0$ otherwise. $\square$

Corollary 1 With rp, plv as in Theorem 8, there exists $\rho' \in \text{R}(S)$ such that, for any $W \in \wp(S)$, we have $\text{sres}_{rp}^{plv}(W) = \text{res}_{\rho'}(W)$.

Not surprisingly, an analogous of Theorem 7, namely Theorem 9, holds for polarising environments over any background set S , provided that $\text{card}(S) > 2$.

Theorem 9 Let $S \in \mathcal{S}, \text{card}(S) > 2$. Then, there exist: $RP \in \wp(\text{RP}(S)), plv \in \text{PLV}(S), \pi \in \text{PROC}(RP, plv)$ such that $\pi \notin \text{PROC}(\mathcal{A})$, for any $\mathcal{A} \in \text{RS}(S)$.

Proof We follow an argument analogous to that in the proof of Theorem 7. Let $\{S \setminus \{x\}, \{x\}\}$ be a partition of S , for some $x \in S$, and let $plv = (S, \{\text{val}, \text{sel}\})$ be such that $\text{val}(x) = -1, \text{val}(y) = 1$ for $y \neq x$ and $\text{sel}(z) = 1$ for $z \in S$. Let then $RP = (S \setminus \{x\}, Y)$ for some $Y \in \wp(S)$. Then, with $W = S$, we have $v_X(S) = (\text{card}(S) - 1) - 1$ and since $\text{card}(S) > 2$, we have $v_X(S) > 0$ by construction. The rest of the proof proceeds as for Theorem 7. $\square$

Remark 5 The condition $\text{card}(S) > 2$ in the proof of Theorem 9 points to an essential difference between polarising environments and relativising ones, as the former do not allow differentiations in the assigned weights, but only in their signs.

5 From immersions to reactions

In this section, we explore some aspects of the immersion of resource-product specifications into polarising environments, pointing to some deeper connection with classical reaction systems. In particular, in Section 5.1 we study the effect of immersing a given rp -spec into polarising environments which form *oppositional pairs* (corresponding to an inversion of the X^-, X^+ sets) or *complementary pairs* (adding to this the inversion of Y^0, Y^+), while Section 5.2 explores the case of reaction systems with disjoint sets of reactants and inhibitors, analogous to sets of reactions of the form (X^+, X^-, Y^+) all derived from immersing a set of rp -specs into a given polarising environment.

Moving from the construction in the proof of Theorem 8, we define a *reaction realisation* operator, rac , such that, for $rp = (X, Y) \in \text{RP}(S), plv = (S, \{\text{val}, \text{sel}\}) \in \text{PLV}(S)$, we have $\text{rac}(rp, plv) = (X^+, X^-, Y^+) \in \text{R}(S)$. For

$B \in \wp(\text{RP}(S))$, we denote by $\text{rac}(B, \text{plv})$ the set $\{\rho \mid \rho = \text{rac}(rp, \text{plv}), rp \in B\} \in \wp(\text{R}(S))$.

Example 4 By taking $S = \{x, y, w, z\}, rp = (\{x, y, w\}, \{w, z\}) \in \text{RP}(S)$, $\text{plv} = (S, \{\text{val}, \text{sel}\}) \in \text{PLV}(S)$ as in Example 3, where $\text{val}(x) = \text{val}(y) = 1$, $\text{val}(w) = \text{val}(z) = -1$ and $\text{sel}(x) = \text{sel}(y) = \text{sel}(w) = 1, \text{sel}(z) = -1$, we obtain $\rho = \text{rac}(rp, \text{plv}) = (\{x, y\}, \{w, z\}, \{x, y, w\}) \in \text{R}(S)$. Note that $\text{en}_\rho(W)$ holds only in $W = \{x, y\}$, which is a strict subset of the sets of states in which rp is weakly/strongly enabled under plv shown in Example 3.

Theorem 10 shows that Theorem 8 does not extend to sets of rp -specifications, so that polarised dynamics define a proper subset of interactive processes (even of context-independent ones).

Theorem 10 *There exists $\mathcal{A} = (S, A) \in \text{RS}(S)$ such that there do not exist $B \in \wp(\text{RP}(S)), \text{plv} = (S, \{\text{val}, \text{sel}\}) \in \text{PLV}(S)$ for which $A = \text{rac}(B, \text{plv})$.*

Proof We prove the thesis by presenting the reaction system $\mathcal{A} = (\{1, 2\}, A)$, where $A = \{(1, 2, 1), (2, 1, 2)\}$. Clearly, this would require that $\text{val} : \{1, 2\} \rightarrow \{1, -1\}$ map both of 1, 2 to both of 1, -1, contradicting its functional nature. $\square$

5.1 Reactions derived from polarising environments

We start here by investigating how the immersion of resource-product specifications into different polarising environments can affect the resulting dynamics. In particular, Definition 14 considers the case of two polarising environments producing opposite polarisations over a common background set. Note that the choice of the selector function is irrelevant to the definition.

Definition 14 (Oppositional pair). For $i \in \{1, 2\}$, let $\text{plv}_i = (S, \{\text{val}_i, \text{sel}_i\}) \in \text{PLV}(S)$ be such that $\text{val}_1(x) = -\text{val}_2(x)$ for $x \in S$. Then, we say that $\Omega = (\text{plv}_1, \text{plv}_2)$ is an *oppositional pair* over S . The set of such pairs is denoted by $\Omega(S)$.

Following the usual convention, it follows that

$$W_{\text{val}_1}^+ = W_{\text{val}_2}^-, W_{\text{val}_1}^- = W_{\text{val}_2}^+.$$

The relation between the dynamics of reaction systems generated by oppositional pairs with identical selector functions is given by Theorem 11.

Theorem 11 *With sel a selector function, let $RP \in \wp(\text{RP}(S))$ and, for $i \in \{1, 2\}$, let $\text{plv}_i = (S, \{\text{val}_i, \text{sel}\}) \in \text{PLV}(S)$, $\text{comp}_+^-(RP, \text{plv}_i)$, with $(\text{plv}_1, \text{plv}_2) \in \Omega(S)$. Then, with $A_i = \{\rho \in \text{R}(S) \mid \rho = \text{rac}(rp, \text{plv}_i), rp \in RP\}$ for $i \in \{1, 2\}$, we have $\text{res}_{A_1}(W) = \text{res}_{A_2}(W^c)$, for $W \in \wp(S)$.*

Proof We first observe that, with $rp \in RP$, if $\rho_1 = \text{rac}(rp, \text{plv}_1), \rho_2 = \text{rac}(rp, \text{plv}_2)$, then we have $R_{\rho_1} = I_{\rho_2}, R_{\rho_2} = I_{\rho_1}$. Now, suppose $\text{en}_{\rho_1}(W)$ holds for some $W \in \wp(S)$, so that $R_{\rho_1} \subseteq W, I_{\rho_2} \cap W = \emptyset$. But then we have $R_{\rho_1} \cap W^c = \emptyset, I_{\rho_1} \subseteq W^c$, and, for the equality above, also $\text{en}_{\rho_2}(W^c)$ holds. Since a bijection exists between A_1, A_2 , such that we can pair reactions from the two sets according to which rp -spec has been used, the result follows. $\square$

Theorem 11 cannot be extended to processes. Indeed, while both of $\text{res}_{A_1}, \text{res}_{A_2}$ would produce the same result set for any pair W, W^c , in general $\text{res}_{A_1}(\text{res}_{A_1}(W))$ need not be equal to $\text{res}_{A_2}(\text{res}_{A_2}(W^c))$. Hence, Definition 15 introduces the notion of *complementary* oppositional pairs:

Definition 15 With $\text{plv}_1 = (S, \{\text{val}_1, \text{sel}_1\}), \text{plv}_2 = (S, \{\text{val}_2, \text{sel}_2\}), (\text{plv}_1, \text{plv}_2) \in \Omega(S)$, we say that $\text{plv}_1, \text{plv}_2$ are *complementary* if we have $\text{sel}_1(x) = 1 - \text{sel}_2(x)$ for $x \in S$. The set of complementary oppositional pairs is denoted by $\Omega^c(S)$.

For pairs in $\Omega^c(S)$ we prove Lemmata 1-3, leading to Theorem 12.

Lemma 1 *With $rp = (X, Y) \in \text{RP}(S)$, let $\text{plv}_i = (S, \{\text{val}_i, \text{sel}_i\}) \in \text{PLV}(S), \rho_i = \text{rac}(rp, \text{plv}_i) \in \text{R}(S)$ for $i \in \{1, 2\}$, with $(\text{plv}_1, \text{plv}_2) \in \Omega^c(S)$. Then, with $W \in \wp(S)$, $\text{en}_{\rho_i}(W)$, we have $\text{res}_{\rho_1}(W) = Y \setminus \text{res}_{\rho_2}(W^c), \text{res}_{\rho_2}(W) = Y \setminus \text{res}_{\rho_1}(W^c)$.*

Proof Since $(\text{plv}_1, \text{plv}_2) \in \Omega(S)$, we know that $\text{en}_{\rho_1}(W) \iff \text{en}_{\rho_2}(W^c)$ and, since $Y_1^+ = Y_2^0 = Y \setminus Y_2^+, Y_2^+ = Y_1^0 = Y \setminus Y_1^+$, the result follows. $\square$

Lemma 2 *With $RP, \text{plv}_1, \text{plv}_2$ as in Lemma 1, let $A_i = \{\text{rac}(rp, \text{plv}_i) \mid rp \in RP\} \in \wp(\text{R}(S))$ for $i \in \{1, 2\}$. Then, we have $\text{res}_{A_1}(W) \subseteq S_1^+, \text{res}_{A_2}(W^c) \subseteq S_2^+$.*

Proof The result follows from Lemma 1, when considering that, with $\rho_1 = \text{rac}((X, Y), \text{plv}_1), \rho_2 = \text{rac}((X, Y), \text{plv}_2)$, we have $\rho_1 \in \text{EN}(A_1, W) \implies Y_1^+ \subseteq \text{res}_{A_1}(W) \subseteq S_1^+, \rho_2 \in \text{EN}(A_2, W^c) \implies Y_2^+ \subseteq$

$\text{res}_{A_2}(W^c) \subseteq S_2^+$, and that $\{S_1^+, S_2^+\}$ is a partition of S by definition of complementarity. $\square$

Lemma 3 *With A_1, A_2 as in Lemma 2, there exists $\text{bij} : A_1 \leftrightarrow A_2$ such that for $\rho_1 = (X_1^+, X_1^-, Y_1^+) \in A_1$ we have $\text{bij}(\rho_1) = \rho_2 = (X_1^-, X_1^+, Y_1^0) \in A_2$.*

Proof The result follows from the construction of A_1, A_2 and the initial observation in the proof of Theorem 11. $\square$

Theorem 12 establishes a correspondence between processes of reaction systems generated by complementary oppositional pairs for some specification.

Theorem 12 *With: $rp \in \text{RP}(S)$; $plv_i = (S, \{val_i, sel_i\})$ for $i \in \{1, 2\}$; and $(plv_1, plv_2) \in \Omega^c(S)$, let $\mathcal{A}_1, \mathcal{A}_2 \in \text{RS}(S)$ derive from $\text{rac}(RP, plv_1), \text{rac}(RP, plv_2)$ respectively. Then, for $\pi_1 \in \text{PROC}(\mathcal{A}_1), |\pi_1| = n$, there exists $\pi_2 \in \text{PROC}(\mathcal{A}_2), |\pi_2| = n$, such that, with $\sigma_{\pi_1}[i] = W$, we have $\sigma_{\pi_2}[i] = W^c$, for $i \in \{0, \dots, n\}$.*

Proof For Lemmata 1–3, every reaction ρ_1 contributing to $\text{res}_{A_1}(W)$ produces a subset of Y_1^+ , while $\text{bij}(\rho_1)$ contributes to $\text{res}_{A_2}(W^c)$ a subset of $Y_2^+ = Y_1^0$, so that $\text{res}_{A_1}(W) \cap \text{res}_{A_2}(W^c) = \emptyset$. We can now proceed to the proof by constructing π_2 in an inductive way. First, for $\kappa_{\pi_1}[0] = (D_0^1, C_0^1, W_0)$, we take $\kappa_{\pi_2}[0] = (D_0^2, C_0^2, W_0^c)$, for some choice of D_0^2, C_0^2 . After that, let $(\kappa_{\pi_1}[i], \kappa_{\pi_1}[i+1])$ be the $i+1$ -th step in π_1 , for $i \in \{0, \dots, n-1\}$, and assume that, with $\kappa_{\pi_2}[i] = (D_i^2, C_i^2, W_i^2)$, we have $W_i^2 = (W_i^1)^c$. For the Lemmata above, we have $\delta_{\pi_2}[i+1] = (\delta_{\pi_1}[i+1])^c$. By taking $\gamma_{\pi_2}[i+1] = S \setminus (\gamma_{\pi_1}[i+1] \cup \delta_{\pi_1}[i+1] \cup \delta_{\pi_2}[i+1])$, the result follows for all steps with $\delta_{\pi_1}[i] \neq \emptyset$. For all other steps, since $\delta_{\pi_1}[i] = \emptyset \iff \delta_{\pi_2}[i] = \emptyset$, we have $\sigma_{\pi_1}[i] = \gamma_{\pi_1}[i], \sigma_{\pi_2}[i] = \gamma_{\pi_2}[i]$ and the result follows by taking $\gamma_{\pi_2}[i] = (\gamma_{\pi_1}[i])^c$. $\square$

Corollary 2 *With $\mathcal{A}_1, \mathcal{A}_2$ as above, let $\pi_1 \in \text{CIPROC}(\mathcal{A}_1)$. Then, there exists $\pi_2 \in \text{CIPROC}(\mathcal{A}_2)$ such that $\delta_{\pi_2}[i] = (\delta_{\pi_1}[i])^c$, for $i \in \{0, \dots, n\}$.*

5.2 Polarised reaction systems

Given a set of resource-product specifications RP , any set of reactions derived from RP via a compatible polarising environment under the rac operator enjoys the *polarisation* property described in Theorem 13, the proof of which is immediate. Note that this property is independent of the selector function.

Definition 16 sets out the reaction systems with this property.

Theorem 13 *With $RP \in \wp(\text{RP}(S)), plv = (S, \{val, sel\}) \in \text{PLV}(S), \text{comp}^+(RP, plv)$, let $A = \{\rho \in R(S) \mid \exists rp \in RP : \rho = \text{rac}(rp, plv)\}$. Then $R(A) \cap I(A) = \emptyset$.*

Definition 16 (Polarised reaction system). With S ; $\mathcal{A} = (S, A) \in \text{RS}(S)$, we say that $\mathcal{A}$ is a *polarised reaction system* over S if we have $R(A) \cap I(A) = \emptyset$. The set of polarised reaction systems over S is denoted by $\text{PRS}(S)$.

Although limited in form, polarised reaction systems maintain the same expressive power as classical ones. Indeed, by Theorem 14, the behaviour of any reaction system can be simulated by that of some polarised system.

Theorem 14 *For $\mathcal{A} \in \text{RS}(S)$, there exist: $S' \in \mathcal{A}' \in \text{PRS}(S')$; $f : \wp(S') \rightarrow \wp(S)$, s.t., for $\pi \in \text{PROC}(\mathcal{A})$, there exists $\pi' \in \text{PROC}(\mathcal{A}')$ with $\sigma_\pi = f(\sigma_{\pi'})$.*

Proof We construct $S' = \{\hat{x}, \check{x} \mid x \in S\}$ (using $\widehat{W}, \check{W}$ to stand for $\{\hat{x} \mid x \in W\}, \{\check{x} \mid x \in W\}$, respectively); define $\mathcal{A}' = (S', A')$ with $A' = \{(\widehat{R}_\rho, \check{I}_\rho, \widehat{P}_\rho \cup \check{P}_\rho) \mid \rho \in A\}$; and take f to be given, for $W' \in \wp(S')$, by: $f(\widehat{W}_1 \cup \check{W}_2) = W_1 \cup W_2$, if $W' = \widehat{W} \cup \check{W}$, and $f(W') = \emptyset$, otherwise. for $\widehat{W}_1, \check{W}_2 \in \wp(S')$. Indeed, for $W \in \wp(S)$ and with $\text{res}_A(W) = D \neq \emptyset$, we have $\text{res}_{A'}(\widehat{W} \cup \check{W}) = \widehat{D} \cup \check{D}$. But now, from $R_\rho \subseteq W, I_\rho \cap W = \emptyset$, we obtain $\widehat{R}_\rho \subseteq \widehat{W} \subseteq W, \check{I}_\rho \cap \check{W} = I_\rho \cap W = \emptyset$, and the thesis follows by taking $\kappa_{\pi'}[0] = (\widehat{W}_0 \cup \check{W}_0, \emptyset, \widehat{W}_0 \cup \check{W}_0)$ and iterating the application of $\text{res}_{A'}$ for the length of π , with $\gamma_{\pi'}[i] = \widehat{C}_i \cup \check{C}_i$ if $C_i \cap (D_i)^c \neq \emptyset$, and $\gamma_{\pi'}[i] = \emptyset$ otherwise. The result holds for any π' such that $\delta_{\pi'}[0] \cup \gamma_{\pi'}[0] = \sigma_{\pi'}[0] = \widehat{W}_0 \cup \check{W}_0$. $\square$

Remark 6 For $\pi \in \text{CIPROC}(\mathcal{A}')$, one can actually restrict the process to be over $\wp(\widehat{S}')$, and revise the definitions of A' and f accordingly.

In what follows, Theorem 15 establishes the relation with polarising environments, while Theorems 16 and 17 respectively provide an analogous of Theorem 11 for polarised reaction systems derivable from an oppositional pair of polarising environments, and an analogous of Theorem 12 for polarised reaction systems derivable from a complementary oppositional pair of polarising environments.

Theorem 15 *For $\mathcal{A} \in \text{PRS}(S)$ there exist $S' S', RP \in \wp(\text{RP}(S'))$, $plv = (S', \{val, sel\}) \in \text{PLV}(S'), f : \wp(S') \rightarrow \wp(S)$ such that, for $\pi \in \text{PROC}(\mathcal{A})$, there exists $\pi' \in \text{PROC}_s(RP, plv)$ with $\sigma_\pi = f(\sigma_{\pi'})$.*

Proof We take both of S', f as in the proof of Theorem 14, with val given by $val(\hat{x}) = 1$, for $x \in R(A)$ and

$val(\check{x}) = -1$, for $x \in I(A)$, and sel given by $sel(x) = 1$ for $x \in S'$. The rest of the proof proceeds as for Theorem 14. $\square$

Theorem 16 *Let $\mathcal{A}, \mathcal{A}' \in \text{PRS}(S)$, $card(A) = card(A')$, $bij : A \leftrightarrow A'$ be such that, for $\rho \in A$, $\rho' = bij(\rho) \in A'$, we have $R_\rho = I_{\rho'}$, $I_\rho = R_{\rho'}$, $P_\rho = P_{\rho'}$. Then, for $W \in \wp(S)$, we have $res_A(W) = res_{A'}(W^c)$.*

Proof For $\rho \in A$, $W \in \wp(S)$, we have $res_\rho(W) = P_\rho \neq \emptyset$ if and only if $R_\rho \subseteq W$, $I_\rho \cap W = \emptyset$, which is equivalent to having $I_\rho \subseteq W^c$, $R_\rho \cap W^c = \emptyset$. But since, with $\rho' = bij(\rho)$, the above is the condition for enabling ρ' and producing $P_{\rho'} = P_\rho$, the result follows, taking into account the cumulative nature of res_A . $\square$

Corollary 3 *With A, A', W as above, we have $EN(A', W^c) = bij(EN(A, W))$.*

Theorem 17 *Let $\mathcal{A}, \mathcal{A}' \in \text{PRS}(S)$, $bij : A \leftrightarrow A'$ be as in Theorem 16, with the additional condition $P_{\rho'} = P_\rho^c$. Then, for $\pi \in \text{PROC}(\mathcal{A})$, there exists $\pi' \in \text{PROC}(\mathcal{A}')$, $|\pi| = |\pi'|$, such that, for $i \in \{0, \dots, |\pi|\}$, we have $\sigma_\pi[i] = (\sigma_{\pi'}[i])^c$.*

Proof We observe that the equality $EN(A', W^c) = bij(EN(A, W))$ from Corollary 3 is preserved under the new version of $P_{\rho'}$. Suppose now that $\sigma_{\pi'}[i] = (\sigma_\pi[i])^c$ holds at step i . Then, we would have $\delta_{\pi'}[i+1] = (\delta_\pi[i+1])^c$ and by taking $\gamma_{\pi'}[i+1] = (\gamma_\pi[i+1])^c$ we would obtain $\sigma_{\pi'}[i+1] = (\sigma_\pi[i+1])^c$. By taking $\sigma_{\pi'}[0] = (\sigma_\pi[0])^c$, the thesis follows by induction. $\square$

Corollary 4 *With π, π' as above, we have $\eta_{\pi'}[i] = bij(\eta_\pi[i])$ for $i \in \{0, \dots, |\pi|\}$.*

Since no x in $P(A) \setminus M(A)$ is relevant to the enabling of any reaction in either of A, A' for any $W, W^c \in \wp(S)$ from Theorem 17, we also obtain Corollary 5.

Corollary 5 *With $\mathcal{A}, \mathcal{A}' \in \text{PRS}(S)$, $bij : A \leftrightarrow A'$ as in Theorem 16, let $P_{\rho'} = M(A) \setminus P_\rho$, for $\rho \in A$. Then, for $\pi \in \text{PROC}(\mathcal{A})$, there exists $\pi' \in \text{PROC}(\mathcal{A}')$, $|\pi| = |\pi'|$ such that, for $i \in \{0, \dots, |\pi|\}$, we have $\eta_{\pi'}[i] = bij(\eta_\pi[i])$.*

6 Modelling examples

We describe here some relevant cases of modelling with positive and polarising evaluating environments to model arbitrary processes in the first two cases and context-independent processes in the last case.

In particular, the example of Section 6.1 discusses the influence of environment, acidic or alkaline, in digestion processes through positively valued environments. Then, the example of Section 6.2 presents a case where environmental conditions change the effect of interaction among species, whereas the example in Section 6.3 shows how polarising environments allow the modelling of chemical equations, with the environment steering the direction of the reactions, and limiting their applicability.

All of the examples also give some insight into the difference between modelling through reaction systems and using evaluating environments.

6.1 Influence of environment on digestion

We give a brief account of some phenomena in protein metabolism (see Kageyama 2002; Janiak 2016).

The digestion of proteins (ptn) involves the proteases pepsin (pep) and trypsin (trp), to perform their conversion to proteoses (prt) and peptones (tpn), or polypeptides (ply), respectively. The first conversion process is mediated by pepsin and occurs in the gastric acid environment, while the second one is mediated by trypsin and occurs in the pancreas alkaline environment. Moreover, their inactive forms, pepsinogen (ppg) and trypsinogen (tpg), are only secreted and activated in the proper environments, while they remain inactive in the opposite ones. The activation process requires in both cases the arrival of some signal, typically some food substance to be digested (fds), in order to avoid self-digestion of the tissue in which the precursors are secreted. Specific inhibitors for their activities are, among others, alginates (alg) for pepsin, and plant-derived protease inhibitors (pdi), for trypsin. Also the activation process can be inhibited, for example by pepstatin (pst) for the reaction transforming ppg into pep and enteropeptidase inhibitors (ent) for the reaction transforming tpg into trp.

Hence, we encode the relevant transformations on the background set

$$S = \{\text{fds}, \text{ppg}, \text{tpg}, \text{pep}, \text{trp}, \text{ptn}, \text{prt}, \text{tpn}, \text{ply}, \text{alg}, \text{pdi}, \text{pst}, \text{ent}\}$$

through the set of reactions

$$A = \{(\{\text{fds}, \text{ppg}\}, \text{pst}, \text{tpn}), (\{\text{fds}, \text{tpg}\}, \text{ent}, \text{trp}), (\{\text{pep}, \text{ptn}\}, \text{alg}, \{\text{pep}, \text{prt}\}), (\{\text{trp}, \text{ptn}\}, \text{pdi}, \{\text{trp}, \text{ply}\})\}.$$

Now, it is important to observe that these reactions are all meant to occur in the proper environment, with low pH (acidic, l) for pepsin-related activities and high pH (alkaline, h) for trypsin-related activities, and are inactivated otherwise.

Hence, we model the in/activation of these processes in un/suitable environments via $pev_l = (S, \{val_l\})$, $pev_h = (S, \{val_h\}) \in PEV(S)$, defined as:

- $val_l(x) = val_h(x) = 0$ for $x \in \{fds, ptn, prt, tpn, ply\}$ (food or proteins alone will not start a reaction and the final products are not relevant for enabling);
- $val_l(ppg) = val_l(pep) = val_h(tpg) = val_h(trp) = 1$, $val_h(ppg) = val_h(pep) = val_l(tpg) = val_l(trp) = 0$ (ph-specific reactants need to be present in the proper environment and are irrelevant in an unsuitable environment).

Finally, we have:

- $val_l(pst) = val_l(alg) = val_h(ent) = val_h(pdi) = 1$;
- $val_h(pst) = val_h(alg) = val_l(ent) = val_l(pdi) = 0$,

as the presence of ph-specific inhibitors is relevant only in a suitable environment.

Now, strong enabling of the reactions for proteases activation or metabolic effects is possible only in the proper environment. Note that weak enabling would allow reactions to produce proteases or metabolites (but only in the proper environment) even in the absence of substance matter to feed the process (but not in the absence of proteases or their precursors), if no specific inhibitor is present, possibly reflecting some malfunctioning of the system.

We can contrast the setting of this process in the framework of positively evaluating environments, with what would be needed in the classical setting, barring considerations on the fact that in both cases it can only be sustained by input from the environment, as neither food nor proteins are produced by internal reactions. Indeed, in the standard setting, modelling the influence of acidity on the reactions would require to have an explicit encoding of the pH level in the background set and its sustained presence in the state, either by continuous and consistent input from the environment, or through reactions of the form $(H, \#, H)$, for $H \in \{l, h\}$ and $\#$ some dummy entity. Moreover, either the adversarial value of H should be included as inhibitor, or the reinforcing value should be included as reactant, making sure that the two entities never occur together in any state.

This suggests the possibility of systematically substituting complex encodings by proper definitions of the evaluator functions, rendering entities relevant only in proper environments and inert in other ones.

Another obvious solution would be the construction of “pH-specific” reaction systems, so that reactions pertaining to pepsin- or trypsin-based processes would reside in different systems. Of course, while not requiring modifications to

the reactions or constraints on the environment, this would affect the possibility of extending such systems with reactions occurring in both environments, which would require the duplication of the “pH-agnostic” reactions in both systems.

6.2 Effects of environment on plant growth

The presence of nurse plants create gradients in the area covered by them, with more favourable conditions for growth at the centre of their canopy, and more stressful ones at its edge, due to the different level of protection from abiotic stress, e.g., UV rays. However, some species of plants can perform better (i.e., produce more biomass) in the less favourable environment, by activating some form of reciprocal facilitation for the growth of neighbouring same-species individuals, while maintaining a competitive behaviour in the more favourable environment, with an overall effect of reduction of the biomass for that species in terms of a minor growth for each individual.

Such an effect emerges in the experiment reported in Al-Namazi et al. (2017), where these phenomena were observed, in the arid conditions of western Saudi Arabia, for different distributions of four species of herbaceous plants (*Farsetia aegyptia*, *Salvia aegyptiaca*, *Fagonia indica*, and *Indigofera spinosa*), in micro-habitats characterised by a gradient in the canopy coverage provided by *Acacia gerrardii* (stress increases with the distance from the centre of the canopy). The authors studied neighbouring effects on the presence of same-species plants for the four species, finding that while all of the species exhibited competitive behaviour among neighbours in the centre of the canopy (favourable soil conditions), the last two species moved to a facilitative behaviour towards the edge (more stressful conditions).

While we do not intend to replicate the quantitative results in Al-Namazi et al. (2017), we can qualitatively model the overall picture by assuming that the soil provides nutrients for all the species, and defining the effect of the presence of other individuals in different environments on the growth of one species, in terms of biomass.

First, with $G = \{sa, fi, fa, is\}$ (from the initials of the four species), we define $S = \bigcup_{sp \in G} \{sp, [sp, +], [sp, -], [sp, sp]\} \cup \{ntr, \#\}$, where:

- $sp \in G$ represents the presence of biomass for the corresponding species;
- $[sp, +]$, $[sp, -]$ indicate an increase or, respectively, decrease of its biomass;
- $[sp, sp]$ indicates the presence of other individuals of sp ;
- ntr represents generic nutrients provided by the environment; and

- # is a dummy entity used so that $S^- \neq \emptyset$.

Then, the interactions which increase/decrease of the biomass of a species sp in the presence of other individuals are modelled by the set of rp -specifications $RP = \bigcup_{sp \in G} \{(\{sp, [sp, sp], \#\}, \{sp, [sp, sp], [sp, +], [sp, -]\}), (\{sp, ntr, \#\}, \{sp\})\}$.

So, this specification prescribes in its resource part the presence of various individuals of the same species, whereas the product part lists the possibility that all individuals are preserved, while the overall volume of the biomass can increase or decrease, depending on the characteristics of the environment.

Now, with $plv_C = (S, \{val_C, sel_C\}), plv_E = (S, \{val_E, sel_E\}) \in PLV(S)$ respectively modelling the centre and the edge of the canopy, we have $val_C(x) = val_E(x) = 1$, for $x \in S \setminus \{\#\}$, and $val_C(\#) = val_E(\#) = -1$.

Moreover, we have $sel_C(sp) = sel_C([sp, sp]) = sel_E([sp, sp]) = sel_C([sp, -]) = 1, sel_C([sp, +]) = 0$ for $sp \in G$ (as we preserve the presence of all the individuals of sp under all conditions, but reduce its overall biomass in favourable environments). Additionally, for $x \in \{fa, is\}$ we have $sel_E([x, +]) = 1, sel_E([x, -]) = 0$, and, for $x \in \{fi, sa\}$, we have $sel_E([x, +]) = 0, sel_E([x, -]) = 1$.

In other words, each rp -spec in RP is executed in both environments, resulting in an increase of biomass only for *Fagonia indica*, and *Indigofera spinosa* at the edge of the canopy, as they recur to facilitation under harsh conditions. In all other cases competition prevails, reducing the overall biomass for each species.

In any case, for $\pi \in PROC(RP, plv_C) \cup PROC(RP, plv_E)$ with initial configuration $\kappa_\pi[0] = (D_0, C_0, W_0)$ such that $sp, ntr \in W_0, \# \notin W_0$, the presence of a biomass $sp \in \{fa, is, fi, sa\}$ will be preserved as long as the environment supplies nutrients; that is to say, for $i \in \{0, \dots, |\pi|\}$, we have $\{sp, ntr\} \subseteq \sigma_\pi[i], \# \notin \gamma_\pi[i] \Rightarrow sp \in \delta_\pi[i+1]$.

Analogously, the presence of neighbouring individuals, as modelled by $[sp, sp]$, will be preserved along a process once $[sp, sp]$ appears in a state (either from the initial state, or by insertion into the environment), provided that sp is already in that state. In this case, also the presence of sp is preserved through the process. Formally, under the same initial conditions on $\kappa_\pi[0]$, for $i \in \{0, \dots, |\pi|\}$, we have $\{sp, [sp, sp], ntr\} \subseteq \sigma_\pi[i], \# \notin \gamma_\pi[i] \Rightarrow \{sp, [sp, sp]\} \subseteq \delta_\pi[i+1]$.

We can compare this solution with the usage of positive evaluating environments, extending S to include E, C (for centre and edge again) and defining the set of reactions $\{(\{sp, [sp, sp], E\}, \#, \{sp, [sp, sp], [sp, +]\}) \mid sp \in \{fi, is\}\} \cup \bigcup_{sp \in G} \{(\{sp, [sp, sp], C\}, (\{sp, ntr\}, \#, \{sp, [sp, sp], [sp, -]\}))\}$.

Then, we define $pev_C = (S, \{val_C\}), pev_E = (S, \{val_E\}) \in PEV(S)$ given by $val_C(\#) = val_E(\#) = val_C(ntr) = val_E(ntr) = 2$, $val_C(x) = val_E(x) = 1$, for $x \in \{S\} \setminus \{ntr, \#\}$, and $val_C(C) = val_E(E) = 1, val_C(E) = val_E(C) = 0$. In this way, the preservation of sp in each environment is still guaranteed, as well as the reduction of its overall biomass in the presence of fellow individuals, while biomass would be increased only for fi, is in harsh environments.

6.3 Modelling chemical equations with polarising environments

A chemical equation is given by a pair of reactions which keep transforming two sets of molecules into each other, possibly producing or consuming heat with each reaction. Given a certain amount of material supporting the reactions, and assuming the environment does not influence the reactions' relative velocities, the reciprocal ratio of the two sets will stabilise at some value k , meaning that both reactions will happen at a velocity maintaining this ratio constant.

An example of such an equation is $N_2 + 3H_2 \rightleftharpoons 2NH_3$, transforming nitrogen and hydrogen into ammonia, and vice versa. In this case $N_2 + 3H_2 \rightarrow 2NH_3$ is exothermic (i.e., producing heat) and $N_2 + 3H_2 \leftarrow 2NH_3$ is endothermic (i.e., consuming heat). Hence, a high environmental temperature will favour the right-to-left direction, and a low temperature will favour the opposite one.

To situate chemical equations within our approach, we represent concentrations of molecules in terms of their distance from the equilibrium, and assume that the amount of heat generated, in one direction, or absorbed, in the other direction, is the same.

In particular, we form a background set with entities which encode the groups of molecules appearing on the sides of the equation as l, r , and the distance of their concentration from the equilibrium by positive integers, using $\uparrow, \downarrow$ to indicate if they are below or above this equilibrium, respectively. For example, $[l, \downarrow, 2]$ indicates that 2 more cycles of reactions are required to reduce the current concentration of $N_2 + 3H_2$ to the equilibrium ratio. Then, a state containing this entity will also contain $[r, \uparrow, 2]$, as the concentration of $2NH_3$ will have to increase for those same two cycles to reach the equilibrium. No other entity encoding a relation to the equilibrium can appear in such a state, while, until the equilibrium is reached, we can assume that an entity heat is continuously produced or consumed, depending on which is the prevailing reaction.

Finally, as molecules cannot move so far from the equilibrium that they actually disappear, we assume that concentrations can differ, in a temperature-neutral environment, up to some value v in one direction or the other, and that they

will be equal in size and opposite in sign. Finally, we assume that a high (resp., low) temperature will move the equilibrium point to admit a higher proportion of $2NH_3$ (resp., $N_2 + 3H_2$). Hence, we assume that the admissible distance from equilibrium is limited to some value q (where q represents some extreme condition beyond which the reactions do not occur)³. As a consequence, we have to consider all possible differences in concentration can range (in absolute value) in the range $[1, v + q]$.

As a result, we define the background set $S = S' \cup \{\text{heat}\}$, with $S' = \{[l, \downarrow, v+q], \dots, [l, 0], \dots, [l, \uparrow, v+q], [r, \downarrow, v+q], \dots, [r, 0], \dots, [r, \uparrow, v+q]\}$.

In writing the reactions, we adopt the convention that the notation $X \xrightarrow{S'} Y$ stands for the reaction $(X, S' \setminus X, Y)$. Now, assuming that reactions cannot occur in an environment beyond the conditions set by that environment, we define the set of reactions modelling an equation as $A = A_r \cup A_l \cup A_e$, where:

- $A_r = \{ \{[l, \downarrow, j], [r, \uparrow, j]\} \xrightarrow{S'} \{[l, \downarrow, j-1], [r, \uparrow, j-1], \text{heat}\} \mid j \in \{1, \dots, v+q\} \}$
- $A_l = \{ \{[l, \uparrow, j], [r, \downarrow, j], \text{heat}\} \xrightarrow{S'} \{[l, \uparrow, j-1], [r, \downarrow, j-1]\} \mid j \in \{1, \dots, v+q\} \}$
- $A_e = \{ \{[l, \downarrow, 0], [r, \uparrow, 0]\} \xrightarrow{S'} \{[l, 0], [r, 0]\}, \{[l, \uparrow, 0], [r, 0]\} \xrightarrow{S'} \{[l, 0], [r, 0]\}, [r, \downarrow, 0] \xrightarrow{S'} \{[l, 0], [r, 0]\} \}$

modelling respectively reactions favouring the right-hand side of the equation, the left-hand side of the equation, or keeping the equation in equilibrium.

Now a context-independent process π of length n , for $n > h \geq 2$, starting in a configuration, say, $\kappa_\pi[0] = (\{[l, \downarrow, h], [r, \uparrow, h]\}, \emptyset, \{[l, \downarrow, h], [r, \uparrow, h]\})$, will proceed through a state sequence $\sigma_\pi = \langle \{[l, \downarrow, h], [r, \uparrow, h]\}, \{[l, \downarrow, h-1], [r, \uparrow, h-1], \text{heat}\}, \dots, \{[l, \downarrow, 0], [r, \uparrow, 0], \text{heat}\}, \{[l, 0], [r, 0]\}, \dots, \{[l, 0], [r, 0]\} \rangle$.

For $h = 1$, the state $\{[l, \downarrow, 0], [r, \uparrow, 0], \text{heat}\}$ will be reached after one step, and similarly will be reached in one step, for $h = 0$, the state $\{[l, 0], [r, 0]\}$.

An analogous state sequence will result for a process π' starting from $\kappa_{\pi'}[0] = (\{[l, \uparrow, h], [r, \downarrow, h], \text{heat}\}, \emptyset, \{[l, \uparrow, h], [r, \downarrow, h], \text{heat}\})$, with a state sequence $\sigma_{\pi'}$ ending in $\langle \{[l, \uparrow, 0], [r, \downarrow, 0]\}, \{[l, 0], [r, 0]\}, \dots, \{[l, 0], [r, 0]\} \rangle$. This time the heat will have to be provided by the environment at each step, though.

Based on this, we model the influence of the environmental temperature on the effects of the equation as a polarising valuating environment $plv_k = (S \cup \{\#\}, \{val_k, sel_k\})$, for

some $-q \leq k \leq q$, where $\#$ is a dummy entity needed to ensure $S^- \neq \emptyset$, while k indicates how far from v the environment can move the point of equilibrium, the sign of k stating whether the environment is high-temperature (ratios can only be below v) or low temperature (ratios can only be above v). Of course, $k = 0$ corresponds to a temperature-neutral environment.

Then, val_k , for $k < 0$, is given by $val_k(x) = 1$ for $x \in \{[l, \downarrow, \text{dst}], [r, \uparrow, \text{dst}] \mid \text{dst} \leq \text{abs}(k)\}$, and $val_k(x) = -1$, otherwise, indicating that the environment will favour the hexo-thermic reactions in A_r .

Conversely, for $k > 0$, we have $val_k(x) = 1$ for $x \in \{[l, \uparrow, \text{dst}], [r, \downarrow, \text{dst}] \mid \text{dst} \leq \text{abs}(k)\}$, and $val_k(x) = -1$, otherwise, indicating that the environment will favour the endo-thermic reactions in A_l . Finally, for $k = 0$, we have $val_0(x) = 1$ for $x \in S \setminus \{\#\}$ and $val(\#) = -1$.

Note that we will have $val(\text{heat}) = -1$ in both cases. Since we assume that all states can only have two entities as described above and the optional heat, we will have $v_R(W) = 2, v_I(W) \leq 1$ in any case. For the function sel_k , if $k < 0$, we take $sel_k(x) = 1$ for $x \in \{[l, \downarrow, \text{dst}], [r, \uparrow, \text{dst}] \mid \text{dst} \leq \text{abs}(k)-1\} \cup \{\text{heat}\}$, and $sel_k(x) = 0$, otherwise. Then, if $k > 0$, we take $sel_k(x) = 1$ for $x \in \{[l, \uparrow, \text{dst}], [r, \downarrow, \text{dst}] \mid \text{dst} \leq \text{abs}(k)-1\} \cup \{\text{heat}\}$, and $sel_k(x) = 0$, otherwise.

We then complete the model by defining the set of rp -specifications $RP = \{(X \cup \{\#\}, Y) \mid X = M_\rho, Y = P_\rho, \rho \in A\}$. In other words, each rp -spec in RP will mimic a reaction in A . Then, the execution of the immersion of RP in one of the plv_k in a state W will isolate the only specification for which $v_X(W) > 0$, thus replicating a context-independent process in $\mathcal{A} = (S, A)$.

Namely, for $\pi \in \text{CIPROC}(\mathcal{A})$, $|\pi| = n$, with $\kappa_\pi[0] = (\{[l, \downarrow, h], [r, \uparrow, h]\}, \emptyset, \{[l, \downarrow, h], [r, \uparrow, h]\})$, $h \leq q$, for any $k \leq h$, there exists $\pi' \in \text{CIPROC}(RP, plv_k)$, $|\pi'| = n$, such that $\kappa_{\pi'}[0] = \kappa_\pi[0]$ and $\sigma_{\pi'} = \sigma_\pi$. The same holds for $\kappa_\pi[0] = (\{[l, \uparrow, h], [r, \downarrow, h]\}, \emptyset, \{[l, \uparrow, h], [r, \downarrow, h]\})$, with $h \leq q$.

It is to be noted that the usage of polarising environments allows the same set of rp -specs to be used for any environmental condition k departing, within the limit set by q , from the reference v for any given temperature, whereas without this feature one would need a different set of reactions for each possible environment.

³ For simplicity we assume that q is equal in both directions and that it is the same for all temperatures.

7 Related work

As the notions of evaluating environments and resource-product specifications appear, to the best of our knowledge, novel, we have not identified directly relatable literature, but we focus here on possible connections with other work.

In a companion paper (Bottoni et al. 2025), valences are used in the context of multiset reaction systems, i.e., where states are multisets, but the assignment of valences is associated with individual reactions, and not with entities. However, the case is considered where all reactions share the same assignment of valences to entities, in a way analogous to that of positively valuating environments. In this case, drawing also from models of reaction systems based on multisets in Mitrana et al. (2025); Bottoni et al. (2025), the outcome of an application preserves the residual of a state, once the reactants of the enabled reactions are removed from the current state. In Bottoni et al. (2025), a relation between entities is also considered, where inhibitors are targeted towards specific reactants. Hence, also inhibitors are removed, if they are annihilated by the presence of paired reactants. As we rely on standard sets, in our framework, similarly to classical reaction systems, all elements not sustained by the products of reactions are lost. Setting the approach to multisets, we could explore the consequences of the various features discussed there.

Evolving reaction systems (see Ehrenfeucht et al. 2017) can model different environmental conditions by activating different sets of reactions at different steps of the process. However, the selection of a new set of reactions can be either arbitrary or depending on the reached state, and it is not intended to model the environment, but rather evolutive steps in the existence of a system.

Various forms of opposition between reactants/facilitators and inhibitors have been discussed in literature. Apart from works on standard reaction systems on sets and their extension to graphs (Kreowski and Rozenberg 2019), we mention Forbidding-Enforcing systems on strings introduced in Ehrenfeucht and Rozenberg (2003) and further studied by Genova for strings and graphs (see Genova and Jonoska 2012; Genova and Hoozeboom 2017), and promoters/inhibitors for membrane computing (Bottoni et al. 2002). A bridge with membrane computing (Păun 2012; Păun et al. 2013) can indeed be identified in that they assign specific sets of reactions to the environment as defined by the internal of a membrane. In our approach, an environment can derive a set of reactions from a set of *rp-specs*, but it is not directly equipped with any specific set. However, the notion of compatibility could be extended so that an environment can be compatible only with specifications with some given property.

The use of environment as a global regulator of processes can be related to the notion of “ontrol word” in regulated rewriting (see the seminal reference Dassow and Păun 1990). An early example in the standard framework of reaction systems is the modelling of the binary counter, with the environment providing a “bit” at each step (Brijder et al. 2011).

Properties of context sequences with respect to the unfolding of processes, have been studied in different contexts, from predicting the generation of specific entities within a certain number of steps (Barbuti et al. 2016), to studying causalities (Barbuti et al. 2018), defining sequences which generate longest threads of states with some properties (Alhazov et al. 2025), to providing logical formulae for the generation of specific sequences (Meski et al. 2015). It would be interesting to revise such results in the framework of evaluating environments.

Variable conditions in an environment have been studied in Azimi et al. (2014), to consider the evolution of responses to heat shocks occurring with subitaneous increases in temperature, causing misfolding of proteins. The response is mediated by specific heat-shock proteins which facilitate the refolding of the misfolded proteins. When the body temperature returns to normal conditions, the process stops.

8 Conclusions

Leveraging the notions of *reactants*, *inhibitors*, and *products* at the basis of the reaction system computational model, we have introduced a novel framework, giving a more prominent role to the environment, not restricted to contributing context, but actually determining the enabling conditions and the products of reaction specifications.

In particular, an *evaluating* environment establishes the relative *valence* of entities acting as reactants or inhibitors (possibly allowing the application in a state W of reactions which would not be enabled in W according to the standard setting), and determines the outcome of immersing a reaction specification (either an actual reaction or a pair of sets of resources and candidate products) into the environment itself.

From the definition of a particular type (called *polarising*) of environments, we have also derived a special family of reaction systems, where entities in a background set can only play the role of reactants or of inhibitors in each reaction of a system. Although limited in their form, it has been shown that systems formed with such *polarised* reactions can simulate the processes of any generic reaction system.

A number of developments are possible. First, some further characterisation of processes induced by evaluating environments as well as of processes in polarised reaction

systems is in order. Of interest is also the pairing of the latter systems with distinction structures (Bottoni et al. 2025), along the orthogonal dimensions of reactants vs. inhibitors and reaction-produced vs. environment-contributed entities.

Also, we plan to extend the use of evaluating environments and of result-product specifications to the framework of *quantitative* (see Mitrana et al. 2025) and *multiset* reaction systems (see Bottoni et al. 2025). In these models, states are made of multisets rather than sets and the application of a reaction preserves the residual of the state, once valued reactants and inhibitors have been removed. A first usage of valences in these cases has been proposed in Bottoni et al. (2025), where valences are associated with specific reactions, rather than having a global impact prescribed by the environment.

Another possible extension is to further enrich the notion of environment, so that it can also be equipped with a function computing the context contribution based on previous results produced by the system, as in Bottoni et al. (2019), or it can be constituted by neighbours in a network, each hosting a reaction system, while being possibly equipped with different valence functions, as in Bottoni et al. (2020). In this vein, one can devise a notion of *migration* of reaction systems (or of *rp-specs*), together with their state, from one environment to a neighbouring one, so that the same system is subject to different enabling conditions from one environment to another. Of interest can now be *hybrid* networks, where the environments are of different nature (positive, relative, or polarising).

Variations in the *val*, *sel* functions of an evaluating environment could be considered as an alternative to evolving reaction systems in the modelling of situations where a physical environment undergoes state transitions, such as the insurgence, steadiness, and retreating of fever. In other words, with $ev = (S, \mathcal{V}) \in EV(S)$, such that $\mathcal{V}$ contains a set of various evaluators, one could envisage some law to activate them, one at a time, depending on various conditions to be modelled in the evolution of a process. The expressive power of such *evolving evaluators* can then be compared to that of *migrating systems* as conceived above.

Finally, we want to pursue the avenue of research hinted at in the final observations of Section 6.1, i.e., comparing evaluating environments to traditional mechanisms to achieve controllability through the specification of context sequences (e.g., Brijder et al. 2011; Ivanov and Petre 2020; Ballis et al. 2024), as ways of steering interactive processes.

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Data Availability No datasets were generated or analysed during the current study.

Declarations

Competing interests The authors declare no competing interests.

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