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The Impact of REACH on Eco-Innovation: How Perception Misfits on Policy Stringency Matter

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Abstract

This article provides new insights into the impact of various policy designs on firms' innovative activities of substituting dangerous chemicals with less damaging ones. Such a principle of substitution is at the heart of the REACH regulation enacted in 2007 to control potentially dangerous chemicals in the European Union (EU). In recent years, research scientists, government panels, and the popular press have denounced bisphenol-A (BPA) used in food packaging for its developmental effect as an endocrine disruptor. In this article, we develop an agent-based model (ABM) as an explorative tool to investigate how the policy design of REACH can help bring safer substitutes of bisphenols to market. We mimic the main mechanisms underlying REACH, suggest the importance of perceived stringency on eco-innovative activities, and address the issue of possible interaction among the various policy design aspects. The modeling exercise enables an analysis of misfits likely to emerge between objective and perceived stringency of regulation as well as misfits related to divergent perceptions between suppliers and clients. The model outcomes stress that the efficiency of severe regulation depends little on how agents perceive it; objective stringency is self-sufficient to stimulate technology transition. A severe regulation results in a stable oligopoly after experiencing an early but short turbulent phase because of the ban of the dangerous substance. This action calls for an assessment by policy makers of the necessary trade-offs between fast environmental and health benefits, temporary demand mismatches and higher market concentration. By contrast, the impact of a lenient regulation depends sorely on how agents perceive it. In particular, possible misfits in the perception of policy stringency between suppliers and clients may strengthen the efficiency of the regulation or, on the contrary, make it irrelevant. These findings highlight that the way stakeholders perceive the regulatory threat may be a key aspect to consider when fostering technological transition.

Keywords: Technology substitution, perceived stringency, REACH regulation, bisphenols, agent-based model (ABM)
Introduction

The substitution of hazardous chemicals by safer alternatives is one of the principles governing the European chemicals policy of REACH1 (EC 1907/2006). Its implementation takes place through the obligation by manufacturers and importers to apply for authorization before a substance of very high concern (SVHC)2 can be used. Industry is thus motivated to search for alternatives for those substances or uses that pose the highest risk to people and the environment. However, a gap between the intentions of REACH and its implementation has come to light especially when facing substances characterized by systemic risks with epistemic uncertainties and numerous knowledge gaps (such as endocrine disruptors) (Munck af Rosenschöld et al., 2014). Thus various observers have expressed the need for fine-tuning the authorization procedure (ChemSec, 2015; Hansen et al., 2007). This raises the question of a well-designed policy able to promote substitution. A large body of literature has stressed that policy design plays a crucial role in eco-innovation (Jänicke, 2012; Johnstone et al., 2012; Kemp & Pontoglio, 2011). Policy design refers to the way environmental regulation has been designed and implemented to stimulate innovation (OECD, 2011).3 REACH provides a unique ongoing experimental field by enabling the study of how the policy may be well designed to drive radical innovation.

Regarding the methods used to examine the link between eco-innovation and policy, four main bodies of literatures have been employed (Kemp & Pontoglio, 2011): theoretical models of incentives for eco-innovation (Fischer et al., 2003; Milliman & Prince, 1989; among others); econometric studies (Horbach, 2008; Horbach et al., 2013; Jaffe et al., 2002; Kesidou & Demirel, 2012; Vollebergh, 2007); case studies (Ashford et al., 1985; Sartorius & Zundel, 2005); and surveys of firms (Cleff & Rennings, 1999; Johnstone, 2007). In addressing the determinants of eco-innovation, these studies point to the important influence of the type and stringency of environmental regulations in shaping innovation trajectories. However, measuring environmental policy is not so easy. Incorporating design aspects of environmental policy instruments in the econometric analysis and in particular defining a proxy for policy stringency are difficult tasks (Borghesi et al., 2015; Brunnermeier & Cohen, 2003; Kesidou & Demirel, 2012; Rennings, 2000). Beyond those practical questions, these considerations have theoretical and methodological implications. From a theoretical standpoint the objective design of environmental policies and their perception require careful attention when assessing the effect of environmental regulation on eco-innovations. Moreover, the dynamic interaction among different policy design aspects is often lacking, whereas it may affect innovation decisions. From an empirical standpoint we need an approach that can draw insights from the complex mechanisms underlying transition dynamics. As pointed out in Lopolito et al. (2013), an ABM methodology is a relevant tool that is able to disentangle complexity resulting from the interrelation between parts and the collective behavior of a system. In this article, we use an ABM methodology to investigate the fundamental processes involved in the substitution of dangerous chemicals and the role that policy stringency, objectively viewed and individually perceived, can have in driving such processes. We study the coevolution process between a population of suppliers and a population of clients involved in the transition from bisphenol-based materials to bio-based substitution materials. Bisphenols are at the center of controversies regarding the health and environment effects they are likely to pose, thus putting the issue of their substitution at the heart of societal and industry challenges. A

1 The acronym REACH stands for Registration, Evaluation, Authorization, and restriction of CHEmicals.
2 SVHCs include cancer and mutation-causing chemicals, persistent toxins that build up in animals and nature, and hormone-imitating chemicals that can have negative health effects.
3 Relevant aspects of design and implementation have been underlined (Kemp & Pontoglio, 2011, p.34): stringency, predictability, flexibility, differentiation with regard to industrial sector or the size of the plant, timing, credibility of policy commitments to future standards, possibilities for monitoring compliance and discovering noncompliance, enforcement, and combination with other instruments of policy.
A stylized version of the authorization procedure such as envisaged in REACH is given a formal representation. How can REACH, and especially the authorization procedure, be fine-tuned to make bisphenols substitution possible? In this work we aim to address these points gaining ground on the ABM developed in Arfaoui et al. (2014), focusing on how perceived stringency influences technology transition.

As discussed in Section 2, different aspects of the policy design, such as stringency, flexibility, and timing, matter for stimulating eco-innovations but also so does the degree of perceived stringency of the environmental policy. Section 3 presents the model and highlights the main improvements and differences added to the model previously developed in Arfaoui et al. (2014). The simulation enables an analysis of misfits likely to emerge between objective and perceived stringency as well as misfits related to divergent perceptions between suppliers and clients. Results are displayed in Section 4 and discussed in Section 5. A conclusion is provided in Section 6.

1. Literature background

2.1. The interdependence among different policy design aspects

It is now widely acknowledged that policy design is crucial for eco-innovation, and greater attention is given to its different aspects: stringency, flexibility, timing, and so on (EEA report, 2011). Defining each of these aspects is not as easy as expected because they are partly interdependent. For example, stringency is linked with timing, which itself is related to flexibility (Ashford et al., 1985). However, stringency of environmental regulations is critical to spur radical innovations (Ashford et al., 1985; CIEL, 2013; Cleff & Rennings, 1999; Frondel et al., 2008; Ghisetti & Pontoni, 2015; Kesidou & Demirel, 2012) and as such plays a predominant role for eco-innovation. Johnstone (2007) and Johnstone et al. (2012) bring complementary empirical evidence showing that perceived stringency of the policy framework has a positive effect on eco-innovation. Theoretical works (Schmelzer, 1997; Segerson & Micelli, 1997) have also clearly established that the level of ambition of negotiated agreement targets is positively correlated to the degree of credibility of the regulator’s threat and to the environmental stringency of the threat. Stringency and flexibility aspects can have a self-reinforcing action on credibility but they can also play the other way round. Expectations play a crucial role in influencing investor behavior, and establishing credibility takes time. Too stringent a regulation may be pernicious and weaken its credibility notably because of a risk of expected massive noncompliance (Ashford et al., 1985). As well, too flexible a regulation may have counterproductive effects, thus negatively affecting its credibility because firms can try to exploit regulatory discretion to their own advantage (Brunner et al., 2012; Weitzman, 1980). In sum, although empirical studies have stressed the role of policy stringency perception to determine environmental performance, it is largely absent from theoretical models.

Moreover, we know very little about the differences of stringency perception depending on firm size or the position in the supply chain. Oosterhuis et al. (2013) consider the possibility that buyers and suppliers perceive technology uncertainty differently. Similarly heterogeneity of firm perception with respect to policy stringency implies that some clients may confer more credibility on the regulatory threat and the withdrawal of a core substance resulting in the loss of product markets. By contrast, suppliers that lag behind their peers in eco-innovation may not believe in

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4 Brunner et al. (2012) give the example of the periodic update of emission caps in the EU Emissions Trading Scheme. Flexible caps provide firms with an incentive to distort investment decisions in order to signal high compliance costs and prepare the ground for a more lenient cap in subsequent trading periods (Harstad & Eskeland, 2010). A firm’s chance of winning with this strategy increases with its market power, thus carrying the risk of a regulatory capture. Brunner et al. (2012) underline that assessment by firms does not entail a binary choice but rather extends along a continuum between perfectly credible and perfectly incredible. Then the level of perceived credibility by a firm depends on the government’s observable incentives.
the regulatory threat because there are no existing alternatives. As a result, perceived stringency may differ between client and supplier.

Therefore, three propositions follow:

- Policy design aspects are partly interdependent but stringency plays a predominant role, being objectively set or subjectively perceived.
- Perceived stringency of environmental regulation is an important determinant of environmental performance and perception misfits with observable incentives and constraints may arise.
- Perceived stringency is firm-specific and such heterogeneity of perception may depend on the position in the supply chain, thus creating misfits between supplier perception and client perception.

2.2. Objective and perceived stringency in the case of REACH

REACH contains components that contribute to get an objectively stringent regulation but at the same time provides unclear messages to companies from the European Chemicals Agency (ECHA) and the European Commission and may contribute to blurring the way companies view the relative stringency of the chemicals policy. Two mechanisms provide observable commitment devices that confer objective stringency to REACH: the authorization procedure and the extended producer responsibility (EPR). The first implies that companies that wish to continue to put chemicals that are particularly harmful (SVHCs) on the market must apply for special authorization.5 The aim of this authorization is to properly control the risks stemming from these substances and progressively replace them with suitable less hazardous alternatives or technologies that are economically and technically viable.6 The second mechanism (EPR) leads to greater interactions between suppliers and downstream users. Usually downstream users receive information on hazardous substances and mixtures in safety data sheets. With REACH, communication obligations imply that safety data sheets may have exposure scenario(s) such as annexes. Consequently, suppliers and users communicate more under the influence of REACH (CSES, 2012). In total, the obligations under REACH related to authorization or to information in the supply chain are tangible for the regulated industry: these binding aspects are common knowledge for every firm and are supported by sanctions (economic fines and criminal sanctions) and controls (inspections carried out by the competent authorities) (Milieu report, 2010).

However, unclear messages from ECHA and the European Commission or stances that are not supported by facts and tests are likely to distort firms’ perceptions, which therefore may sense differently the objective stringency of such a complex and evolving regulation as REACH. We observe that some companies have expressed concerns regarding the authorization process: “The outcome of recent opinions for authorization has added to the confusion concerning the authorization process and REACH and its intentions. Companies fear that investments in substitution made to comply with REACH may not have been necessary or may even turn to their disfavor” (ChemSec, 2015, p.3). More generally, the search for a compromise between ambitious and realistic goals permeates the whole regulation, especially when considering the issue of substituting dangerous substances. In particular, the granting or refusal of authorization

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5 These substances are proposed for addition to a candidate list after being submitted by member states and the commission. From the candidate list, they await being moved to the “authorization annex”: a list of chemicals that must be phased out, replaced with safer alternatives, or allowed for specialized use if justified. After a substance has been included in the authorization annex, it cannot be placed on the market or used after a given date (sunset date), unless an authorization is granted for their specific use or the use is exempted from authorization.

6 Companies that apply for an authorization to use substances in the authorization annex may include a socioeconomic analysis as part of their application. It contains a description of the risks as well as information on the health and environmental benefits, the associated costs, and other socioeconomic impacts.
is based on the existence of economically and technically viable alternatives and on the proof of an R&D watch for alternatives. The result is that such a conditioned decision may delay the search for new safer alternatives and is more likely to induce incremental innovations rather than radical ones. Additionally, the CSES report (2012) emphasizes that REACH is characterized by some areas of uncertainty in terms of innovation, thus contributing by sending wrong signals. Uncertainty is clearly reinforced by lobbying activities especially strong in the authorization process (CSES, 2012). By trying to divert or undermine the binding aspects of the legislation, industry lobbying affects the perception of stringency and confers ambiguity on the regulatory threat. All in all, these uncertainties have an influence on planning innovation leading to further delayed investments in substituting harmful substances.

2.3. The case of bisphenols: Controversies and ban of BPA products

In recent years, research scientists, government panels, and the popular press have denounced bisphenol-A (BPA) used in food packaging for its developmental effect as an endocrine disruptor. Over the years, the topic of BPA has divided scientists, industry, and regulatory agencies with one side thinking that there are several discrepancies among the studies claiming an effect on health and the other side arguing why, with so much evidence in place, there is even a question of whether BPA should be banned from use in food packaging.

The division in opinion has resulted in different countries' regulatory agencies deciding on different risk-management strategies for BPA. In September 2010, Canada became the first country to declare the compound a toxic substance that is deemed harmful to health and the environment, and in March of the same year Canada banned plastic baby bottles that contain BPA. In April 2010, Denmark was the first European country to follow suit in banning the use of BPA in any food containers for young children. In France, the national agency for food, environmental, and occupational health and safety (ANSES) proposed in September 2012 a more stringent level of classification of BPA as toxic for reproduction. In March 2013, it was adopted by the Committee for Risk Assessment (RAC) of the European Chemicals Agency (ECHA). Moreover, in April 2013 the agency published the results of an assessment of the health risks of BPA. However in January 2015 the European Food Safety Authority (EFSA) concluded “that there is no health concern for any age group from dietary exposure and low health concern from aggregated exposure” (EFSA, 2015, p.183), thus contradicting the previous conclusions made by ANSES, which in the wake has denounced intense lobbying by big plastic producers.

Currently, under REACH, BPA does not meet the criteria of an SVHC and as such is not subject to authorization. Moreover, BPA has not been included on the candidate list for authorization. Controversies and heterogeneity as to national positions adopted against BPA contribute to weaken the threat of phasing out those substances and nurture different perceptions as to the stringency of future policy commitments. Beyond the controversies, the search for alternatives to the family of bisphenols (A, F, and S) is a challenging issue for industry and public authorities. In

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7 Despite significant advances in the study of endocrine disruptors, several controversies have sprung up and continue, including the debate over the existence of non-monotonic dose response curves, the mechanisms of low-dose effects, and the importance of considering critical periods of exposure in experimental design (Vandenberg et al., 2009).

8 Indeed, since 2002, BPA had been categorized within a harmonized European classification as suspected of reproductive toxicity (Category 2). As part of its research and in relation to effects observed and the criteria in regulation 1272/2008 on the classification of chemicals, ANSES proposed classifying BPA as toxic to reproduction in humans (1B) and also suggested opening a debate about whether it should be classified in Category 1A, depending on how the uncertainty in the human data is interpreted.

9 In late March 2013, based on all the available data, the Committee for Risk Assessment (RAC) of the European Chemicals Agency (ECHA) issued a favorable final opinion on the French proposal to list BPA as a Category 1B repro-toxic substance. See https://www.anses.fr/en/content/bisphenol.
the following, we propose an ABM to study the competition between bisphenol-based materials and bio-based substitution materials. More precisely, we focus on substances used for epoxy resins. Applications of epoxy resins are varied in food packaging, paints, and electric and electronic devices (chips). They are used for their protective coating capacity against corrosion and their thermal stability (INERIS, 2010). Following an exploratory perspective, we assume that bisphenol-based epoxy resins are affected by the authorization procedure of REACH because of their endocrine disruptor properties.

3. Modeling competition between bisphenol-based materials and bio-based substitution materials

The basic principles of the model presented here rely on the model described in Arfaoui et al. (2014), which captures the dynamics of supplier-user relationships in the chemical industry and the development of alternative solvents as they compete and respond to regulatory pressures. In the following modeling exercise, we adapt and extend this first model in order to mimic the main mechanisms underlying REACH (authorization and extended producer responsibility) and study their effects on the transition from bisphenol-based materials to bio-based substitution materials.

3.1. The method: Agent-based modeling (ABM)

In their article examining the innovation effects of environmental policy instruments, Kemp and Pontoglio (2011) call for multi-method analysis. Following their proposition we add ABM to the tool box and we propose a model to study the link between policy design and innovation and to better picture policy interaction effects.

To our knowledge, Arfaoui et al. (2014) is the only attempt investigating the effect of REACH on industrial dynamics by developing an ABM. Such a model is in line with a solid tradition of evolutionary models of industrial dynamics (Malerba, 2006; Safarzyńska & van den Bergh, 2010). Assessing the effect of REACH on technological transition requires coping with complex evolving interactions and feedbacks between heterogeneous suppliers and clients (Safarzyńska et al., 2012). By simulating the behavior of heterogeneous agents, technological diversity, and the change in selection environment that result from policy measures, ABM is ideally suited to assess the effect of REACH on technological transition. It enables the modeling of complex evolving systems in order to study how system-level properties emerge from the adaptive behavior of individuals as well as how, in turn, the system affects individuals. As in Arfaoui et al. (2014), the ABM presented in this article is used as a learning tool and is not intended for accurate prediction. The objective is to shed light on the impact of the stringency features of instruments underlying the authorization procedure of REACH on the associated shift to bio-based substitution materials.

3.2. Model description

We specify the equations of the model and the assumptions underlying them.

3.2.1. Agents and technologies

We consider the market of substances used for epoxy resins of food containers (metal foods and beverage cans). We take into account two interacting categories of firms: suppliers (i) and clients (j). Suppliers search for dominant position in the market through innovation and clients pursue

\[ \text{production costs, mark-up pricing, and the entry process of suppliers were endogenized and the modeling of the perception of regulation by agents has been enhanced.} \]
the objective of finding the most satisfying product consistent with their preferences and with their techno-economic constraints. Suppliers develop, produce, and sell to clients products based on particular technologies. Two types ($k$) of product-related technology are considered: bisphenols A, F, and S, called technology T1; and substitution solutions: examples include bio-based epoxy resins, for example, bio-sourced polyphenols, called technology T2 ($k = T1$ or T2). Clients buy and use one type of product (T1 or T2) in their production processes. Each family of substance (T1 or T2) is able to provide a wide range of food containers. However, they radically differ in their capacity to provide long-lasting or resistant containers (different quality performance) and to contain toxic substances with adverse health and/or environmental effects, thus partly determining different prices.11

Products are depicted as multi-characteristic technologies. Each product is described by four attributes: technical quality ($X$), productive efficiency ($Eff$), toxicity ($Tox$), and environmental risk of bioaccumulation ($Bio$).

- Technical quality is a multi-criterion dimension reflecting the performance of the technical attributes of the product during the use phase.12 The higher the value for $X$ is the better the technical quality.
- Productive efficiency represents the firm’s capacity to efficiently use and combine resources and material inputs (productivity, yields, and delays) when producing. The higher the $Eff$ is, the more efficient the firm.
- Toxicity reflects the hazard properties of substances of specific concern because of the long-term and serious effects that they may exert on human health.13 The lower the $Tox$ is, the lower the health risk.
- Bioaccumulation refers to the accumulation of substances in an organism. Bioaccumulation occurs when an organism absorbs a toxic substance at a rate greater than that at which the substance is lost. Thus, the longer the biological half-life of the substance in the environment is, the greater the risk of chronic poisoning, even if environmental levels of the toxin are not very high. The lower the $Bio$ is, the lower the environmental risk.

Depending on the substance embedded in the product, differences will appear in terms of what is currently achievable (initial values) and potential of progress (technological frontier). In the model, initial values as well as extreme limits for each of these variables are set in order to account for these differences and are grounded on empirical data (INERIS, 2014). Each of these attributes is characterized by a potential of improvement that can be exploited by suppliers according to their R&D and innovation activities. The potential of improvement assigned to each attribute is defined by its initial value and its outer limit. Technical performance and productive efficiency are characterized by a maximum limit ($X_{max}$ and $Eff_{max}$), and toxicity and bioaccumulation are characterized by a minimum limit ($Tox_{min}$ and $Bio_{min}$). These limits are assumed to be different depending on the technology: T1 or T2. T2 is a bio-based technology so its outer limits regarding environmental and health characteristics are better than the limits of the conventional technology T1 ($Tox_{minT2} < Tox_{minT1}$ and $Bio_{minT2} < Bio_{minT1}$). However, T1 and T2 also differ in terms of initial values: T2 is an emergent technology and is initially more expensive and less performing in terms of technical quality than T1, but it is much better in terms of toxicity and bioaccumulation. Only T1 is available at the start of the simulation, and sooner or later T2 may be introduced in the market.

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11 See Table 10 of INERIS (2014, p.38).
12 For instance $X$ reflects the protective coating capacity against corrosion, thermal stability, and impact resistance of food containers.
13 For instance, $Tox$ reflects the carcinogenic, mutagenic, or toxic reproduction impact of substances.
3.2.2. Technology portfolio

Only T1 is initially available at the start of the simulation, but suppliers are assumed to search for substitutes and thus to accumulate knowledge about T2 through an R&D watch. The objective is to cumulate sufficient knowledge about this new technology in order to introduce into the market products based on T2 with competitive price and technical quality. Thus, every period suppliers examine the possibility of introducing T2 into the market. They compare an adoption index with a supplier-specific threshold. The adoption index is as follows:

\[ AdIndex^T_2 = K_{lt} + M_{st}^T \]  

where \( M_{st}^T \) represents the total market share of T2. \( K \) stands for the cumulated knowledge stock on T2 derived from the supplier’s technological watch. The probability of introducing T2 positively depends on the cumulated stock of knowledge on T2 and also on how T2 has diffused in the market. The decision of suppliers to produce and sell T2 follows a two-step procedure. First, the supplier compares its adoption index with an adoption threshold under which the firm will not adopt T2. If the adoption index is above the threshold, then the second step determines if the supplier has a sufficient budget to bear the switching costs related to T2. Suppliers that decide to adopt T2 can continue to produce and sell T1; they will have a technology portfolio constituted of T1 and T2. However, suppliers can decide to abandon T1 and focus only on the development of T2. To make this decision, each supplier calculates the share hold by T2 in its total turnover and compares it with a firm-specific threshold that represents the more-or-less risky attitude of each firm toward T2. The higher the share or the lower the threshold is, the higher the likelihood to bet only on T2 and to abandon T1.

3.2.3. R&D activities and innovation

Each period, every firm can accumulate technological knowledge and can improve the product performance in its portfolio by carrying out R&D and innovation activities. Every firm will allocate a certain proportion (\( \delta \)) of its budget (\( B \)) to R&D activities:

\[ RD_{lt} = \delta \times B_{lt} \]  

This global R&D budget is split between T1 and T2 technologies:

\[ RD1_{l,t} = \delta_{T1} \times RD_{lt} \]  
\[ RD2_{l,t} = (1 - \delta_{T1}) \times RD_{lt} \]

where \( \delta_{T1} \) is the share of total R&D allocated to T1. For firms developing only T2, \( \delta_{T1} = 0 \). For firms developing both T1 and T2, \( \delta_{T1} \in [0; 1] \). For firms developing only T1, \( \delta_{T1} \in [0; 1] \) because they devote the other part to a technological watch on T2 (in that case, \( RD2 = RD_{watch} \)).

Technology watch on T2 follows a stochastic process. Success occurs if the following condition is satisfied:

\[ 1 - e^{-\alpha w \times RD_{watch}_{l,t}} \geq u(0,1) \]

where \( \alpha w \) is a scale parameter determining the speed at which the level of the current R&D expenditure enables knowledge accumulation. \( RD_{watch} \) represents R&D expenses allocated to a technological watch on T2. \( u(0,1) \) is a uniform random value selected between 0 and 1. The closer to 1, the more difficult it is to satisfy the condition (5) with a given R&D investment.
If condition (5) is satisfied, new knowledge \( (K) \) on T2 is accumulated and the switching costs \( (SC) \) linked to the potential adoption of T2 decrease:

\[
K_{i,t} = K_{i,t-1} + \alpha_K \times u(0,1) \times (K_{\text{max}} - K_{i,t-1}) \tag{6}
\]

\[
SC_{i,t} = SC_{i,t-1} - \alpha_{\text{sc}} \times u(0,1) \times (SC_{t-1} - SC_{\text{min}}) \tag{7}
\]

where \( \alpha_K \) and \( \alpha_{\text{sc}} \) are scale parameters and \( K_{\text{max}} \) and \( SC_{\text{min}} \) are respectively maximum and minimum limits for \( K \) and \( SC \).

 Suppliers can improve the performance of the product(s) constituting their portfolio through an innovation process similar to the previous procedure. Two steps are considered for each product characteristic \( (X, \text{Eff}, \text{Tox}, \text{Bio}) \). The first step determines if innovation occurs or not. The innovation probability depends on the R&D investment allocated to the technology. Success occurs for T1 if the following condition is satisfied:

\[
1 - \alpha \times R\&D_{1,i,t} \geq u(0,1) \tag{8a}
\]

where \( \alpha \) represents the speed of the innovation process. The same applies to T2:

\[
1 - \alpha \times R\&D_{2,i,t} \geq u(0,1) \tag{8b}
\]

If condition (8a) or (8b) is satisfied, the new value for, respectively, \( X, \text{Eff}, \text{Tox}, \) or \( \text{Bio} \) is:

\[
X_{k,i,t} = X_{k,i,t-1} + \beta_X \times u(0,1) \times (X_{\text{max}} - X_{k,i,t-1}) \tag{9a}
\]

\[
\text{Eff}_{k,i,t} = \text{Eff}_{k,i,t-1} + \beta_{\text{Eff}} \times u(0,1) \times (\text{Eff}_{\text{max}} - \text{Eff}_{k,i,t-1}) \tag{9b}
\]

\[
\text{Tox}_{k,i,t} = \text{Tox}_{k,i,t-1} - \beta_{\text{Tox}} \times u(0,1) \times (\text{Tox}_{k,i,t-1} - \text{Tox}_{\text{min}}) \tag{9c}
\]

\[
\text{Bio}_{k,i,t} = \text{Bio}_{k,i,t-1} - \beta_{\text{Bio}} \times u(0,1) \times (\text{Bio}_{k,i,t-1} - \text{Bio}_{\text{min}}) \tag{9d}
\]

where \( \beta_X, \beta_{\text{Eff}}, \beta_{\text{Tox}}, \) and \( \beta_{\text{Bio}} \) are scale parameters and \( u(0,1) \) is a uniform random value selected between 0 and 1 that reflects the efficiency of the R&D activity and thus affects the innovative outcome. The last term of the equation represents the distance to the technological frontier associated with each product characteristic.

3.2.4. Pricing strategy and profits

The production costs of a given product depend on its attributes \( X, \text{Eff}, \text{Tox}, \) and \( \text{Bio} \).\(^{14}\) The costs function of supplier \( i \) for product \( k \) at time \( t \) is defined as follows:

\[
\text{Cost}_{k,i,t} = \alpha_{\text{Cost}} \times (X_{k,i,t} - A_X) \times (\text{Eff}_{k,i,t} - A_{\text{Eff}}) \times (\text{Tox}_{k,i,t} - A_{\text{Tox}}) \times (\text{Bio}_{k,i,t} - A_{\text{Bio}}) \tag{10}
\]

with \( \alpha_{\text{Cost}}, A_X, A_{\text{Eff}}, A_{\text{Tox}}, \) and \( A_{\text{Bio}} \) technical parameters. According to that cost equation, costs positively depend on technical quality \( (X) \) but negatively depend on toxicity \( (\text{Tox}) \), bioaccumulation \( (\text{Bio}) \), and productive efficiency \( (\text{Eff}) \). In other words, innovation may lead suppliers to improve product quality or to decrease toxicity and bioaccumulation but it has a cost, leading firms to increase their product price (price premium because of quality effect of innovation). Innovation may also lead suppliers to improve their productive efficiency, enabling them to decrease their production costs and to propose lower prices (price decrease because of the efficiency effect of innovation). Because the various innovation effects are independent, the

\(^{14}\) In Arfaoui et al. (2014), costs were represented by an independent variable.
The total net effect on cost may be positive or negative and will depend on the interactions among suppliers, users, and technology.

The price \( P \) is deduced from the production costs by applying a mark-up rate \( \mu \):

\[
P_{k,i,t} = (1 + \mu_{k,i}) \cdot \text{Cost}_{k,i,t} \quad (11)
\]

with \( \mu_{k,i} \) the mark-up rate of supplier \( i \) for product \( k \). This mark-up rate is given by the following equation\(^{15}\):

\[
\mu_{k,i,t} = \left( \frac{M_{k,i,t} - M_{\text{min},k,t}}{M_{\text{max},k,t} - M_{\text{min},k,t}} \right) + HHI_t \quad (12)
\]

with \( M_{k,i,t} \) the market share of supplier \( i \) for product \( k \), \( M_{\text{min},k} \) and \( M_{\text{max},k} \) respectively the minimum and the maximum market share of product \( k \) over suppliers and \( HHI \) the Herfindahl-Hirshman index of concentration. The first part of the equation takes into account the relative market share of firm \( i \) for product \( k \) such that the higher the individual market share\(^{16}\) the higher the mark-up rate. The second part of the equation introduces the aggregate \( HHI \) index of concentration in order to take into account the market power for an industry as a whole. The lower the competitive pressure the higher the opportunity to apply high mark-up rates.\(^{18}\) These two elements may lead to self-reinforcing or counterbalancing effects and in the end to a wide variety of mark-up rates within the industry.\(^{19}\)

The profits of supplier \( i \) are given by the following equation:

\[
\pi_{i,t} = \sum_k (P_{k,i,t-1} - \text{Cost}_{k,i,t-1}) \times Q_{k,i,t} - FC
\]

\[
\Leftrightarrow \pi_{i,t} = \sum_k \mu_{k,i,t-1} \times \text{Cost}_{k,i,t-1} \times Q_{k,i,t} - FC \quad (13)
\]

where \( Q \) is the total number of products sold by the supplier and \( FC \) are the fixed costs.\(^{20}\) The profits increase the budget \( B \) of the supplier. It is determined by the residual budget from the previous period, the profits \( \pi \), and the R&D expenses \( RD \):

For typical suppliers:

\[
B_{i,t} = B_{i,t-1} + \pi_{i,t-1} - RD_{i,t-1} \quad (14a)
\]

For new T2 adopters:

\[
B_{i,t} = B_{i,t-1} + \pi_{i,t-1} - RD_{i,t-1} - SC_{i,t-1} \quad (14b)
\]

---

\(^{15}\) In Arfaoui et al. (2014), mark-up rates are constant and identical for every supplier.

\(^{16}\) Market shares are an indirect assessment of market power: a monopolistic firm that has 100% of the market is expected to have the highest possible market power; conversely, a firm with a tiny share of the market is expected to be unable to exercise much market power.

\(^{17}\) \( HHI \) can range from \( 1/N \) to 1 (\( N \) is the number of firms in the market), moving from a huge number of very small firms to a single monopolistic producer. Increases in the Herfindahl-Hirshman index generally indicate a decrease in competition and an increase of market power, whereas decreases indicate the opposite.

\(^{18}\) We can note that two particular cases can arise: a monopolist firm \( (MS=MS_{\text{min}}=MS_{\text{max}} \text{ and } HHI=1) \) and a competitive situation with equidistribution of market shares \( (MS=MS_{\text{min}}=MS_{\text{max}} \text{ and } HHI=1/N) \). In such cases, the first term of the equation would display a numerator and a denominator equal to 0; to avoid that we set this term equal to the value of the current firm’s market share \( (MS=1 \text{ and } MS=1/N \text{ respectively}) \).

\(^{19}\) Following this equation, the mark-up rate will take any value between 0 and 2.

\(^{20}\) Fixed costs are supposed to be identical for all firms for simplicity reasons. Profits depend on costs, mark-up rates, and prices of the previous period because these variables are computed at the end of each period, after the purchase process of the clients.
where $SC$ are the switching costs resulting from the adoption of T2 (parameter).

3.2.5. Exit and entry

Suppliers with a negative budget $B$ go bankrupt and disappear from the market. Regarding entry, a probability of entry is calculated based on the progress already achieved in the industry$^{21}$:

$$\text{Prob}_{\text{entry}} = \alpha_{\text{entry}} \times (M_{T_{1}}^{t-1} \times \text{Score}_{T_{1}}^{t} + M_{T_{2}}^{t-1} \times \text{Score}_{T_{2}}^{t}) \quad (15)$$

with $\alpha_{\text{entry}}$ a parameter reflecting the maximum probability of entry, $M_{T_{1}}$ and $M_{T_{2}}$ the respective market shares of each technology and $\text{Score}_{T_{1}}$ and $\text{Score}_{T_{2}}$ the variables calculated according to the following equations:

$$\text{Score}_{T_{1}}^{t} = \frac{X_{\text{max}}^{T_{1}} - a_{X_{	ext{min}}^{T_{1}}}}{X_{\text{max}}^{T_{1}} - X_{\text{min}}^{T_{1}}} \times \frac{\text{Eff}_{\text{max}}^{T_{1}} - a_{\text{Eff}_{\text{min}}^{T_{1}}}}{\text{Eff}_{\text{max}}^{T_{1}} - \text{Eff}_{\text{min}}^{T_{1}}} \times \frac{a_{\text{Tox}_{	ext{min}}^{T_{1}}}}{a_{\text{Tox}_{\text{max}}^{T_{1}}}} \times \frac{a_{\text{Bio}_{\text{min}}^{T_{1}}}}{a_{\text{Bio}_{\text{max}}^{T_{1}}}}$$

$$\text{Score}_{T_{2}}^{t} = \frac{X_{\text{max}}^{T_{2}} - a_{X_{	ext{min}}^{T_{2}}}}{X_{\text{max}}^{T_{2}} - X_{\text{min}}^{T_{2}}} \times \frac{\text{Eff}_{\text{max}}^{T_{2}} - a_{\text{Eff}_{\text{min}}^{T_{2}}}}{\text{Eff}_{\text{max}}^{T_{2}} - \text{Eff}_{\text{min}}^{T_{2}}} \times \frac{a_{\text{Tox}_{\text{min}}^{T_{2}}}}{a_{\text{Tox}_{\text{max}}^{T_{2}}}} \times \frac{a_{\text{Bio}_{\text{min}}^{T_{2}}}}{a_{\text{Bio}_{\text{max}}^{T_{2}}}}$$

with $X_{\text{max}}$, $\text{Eff}_{\text{max}}$, $\text{Tox}_{\text{min}}$, and $\text{Bio}_{\text{min}}$ the outer limits of the respective characteristics of T1 and T2; $a_{X}$, $a_{\text{Eff}}$, $a_{\text{Tox}}$, and $a_{\text{Bio}}$ the industry average performance; and $X_{0}$, $\text{Eff}_{0}$, $\text{Tox}_{0}$, and $\text{Bio}_{0}$ the initial values of these characteristics. The variables $\text{Score}$ reflect the technological progress made by the industry on the different characteristics of each technology. According to equations (15), (16a), and (16b), the higher the technological progress made by the industry is, the lower the technological potential to be exploited and so the lower the probability to enter. If the entry draw is a success, a new competitor enters the market. The technology portfolio and the product characteristics of the new entrant are fixed by copying an incumbent. The imitated supplier is randomly selected with probabilities proportional to the incumbents’ market shares. We assume that the entrant has an absorptive capacity that enables it to copy the attributes of the imitated with more or less success: the new supplier can underperform or inversely overperform in comparison with the imitated incumbent.$^{22}$

3.2.6. Product purchase

At the very first period of the simulation run, each client ($j$) has to select a product through a purchase procedure, which is composed of the three following steps:

1. Each client randomly chooses one product characteristic. The probability of a characteristic being chosen is proportional to the client-specific preferences of technical quality of products ($\text{prefX}$), price ($\text{prefP}$), toxicity ($\text{prefTox}$), and environmental risk of bioaccumulation ($\text{prefBio}$).$^{23}$

2. The client scans all the products marketed by each supplier and gives them a score proportional to the selected characteristic in step 1. We consider the following score functions ($U$) when the selected product characteristic is respectively technical quality ($X$), price ($P$), toxicity ($\text{Tox}$), or bioaccumulation ($\text{Bio}$):

$$U_{k,i,t}^{j} = (X_{k,i,t-1} - Z_{X}) \times (M_{S_{lt-1}} + u(0,0.1))^2 \quad (17a)$$

$^{21}$ Arfaoui et al. (2014) considers that any firm exiting the market is automatically replaced by a new entrant so that the number of suppliers is kept constant over the whole time period.

$^{22}$ The initial budget ($B$), knowledge stock ($K$), and switching costs ($SC$) of the new entrant are functions of the industry average.

$^{23}$ $\text{prefX}$, $\text{prefEff}$, $\text{prefTox}$, and $\text{prefBio}$ are initially randomly chosen between 0 and 1.
\[ U_{k,i,t}^j = (Z_P - P_{k,t-1}) \times (Ms_{t-1} + u(0,0.1))^z \] (17b)

\[ U_{k,i,t}^j = (Z_{Tox} - Tox_{k,t-1}) \times (Ms_{t-1} + u(0,0.1))^z \] (17c)

\[ U_{k,i,t}^j = (Z_{Bio} - Bio_{k,t-1}) \times (Ms_{t-1} + u(0,0.1))^z \] (17d)

\( Z_X, Z_P, Z_{Tox}, \text{and } Z_{Bio} \) are technical parameters used only to avoid negative terms in the score calculation. \( u(0,0.1) \) is drawn from a uniform distribution with values between 0 and 0.1 to avoid \( U = 0 \) when the market share (\( Ms \)) of the product is null. The parameter \( z \) can be interpreted as a bandwagon effect reflecting imitation behaviors.

3. The client randomly selects one product. The probability of a product being chosen is proportional to its score \( U \) calculated in step 2. Each client is also supposed to be limited by economic and technical constraints, so we assume a reserve price and a minimum technical quality requirement for each client. If the selected product does not satisfy one of these constraints, it is discarded and the client selects another product following the same procedure. If there is no product that satisfies these constraints, the client does not buy and own any product during the period.

Once a product is selected by a client, the corresponding supplier registers a sale. Each client is assumed to use one single product at the same time and to renew its purchase every period. The client can choose to keep the same supplier or to leave the supplier following the two-step process:

1. Each client randomly chooses one product characteristic. The probability of a characteristic being chosen is proportional to the client-specific preferences \( pref_X, pref_P, pref_{Tox}, \text{and } pref_{Bio} \).

2. When the selected characteristic in step 1 is respectively \( X, P, Tox, \text{or } Bio \), the client will make the following decision: if \( X_{k,t-1}^j \leq Tol \times \max X_{k,t-1}, P_{k,t-1}^j \geq Tol \times \min Price_{k,t-1}, Tox_{k,t-1}^j \geq Tol \times \min Tox_{k,t-1}, \text{or } Bio_{k,t-1}^j \geq Tol \times \min Bio_{k,t-1}, \) the client leaves his or her current supplier and chooses another one through the purchase procedure; otherwise, the client keeps the same supplier. \( X, P, Tox, \text{and } Bio \) are the attributes of the product owned by the client \( j \), and \( \max X, \min Price, \min Tox, \text{and } \min Bio \) are the best industry performances achieved. \( Tol \) is a random number from a uniform draw allowing a certain zone of tolerance according to which a client may accept variation within a range of performances.

At the end of the purchase process, the total number of sales and the market share of each supplier are calculated.

3.2.7. Regulation mechanisms

The two main mechanisms underlying REACH are taken into account: authorization process and extended producer responsibility.

The authorization procedure concerns dangerous substances that need a permit before being used in the market. The permit is authorized for a certain time period only if no economically and technically viable alternatives exist and if the firm proves to carry out research activities on alternatives. Otherwise the permit is not granted and the dangerous substance is prohibited after the so-called sunset date. In sum, authorization takes place sequentially and involves revisable guidelines in order to force the search for viable alternatives through an R&D watch. In the model, the authorization process is characterized by a sequential checking procedure based on a
sunset date \( T_{\text{sun}} \) associated with revision dates and target thresholds \( X^*, Eff^*, \) and \( \alpha_{\text{Watch}} \). When the current period is the sunset date \( (t = T_{\text{sun}}) \), the authorization process occurs. It consists of comparing the average technical performance and the average productive efficiency of T2 with the techno-economic performance targets, respectively \( X^* \) and \( Eff^* \). These targets serve as screening devices in the hand of the public agency (ECHA) to check whether economically and technically viable alternative substances (T2) exist and if so to ban T1 after the cutoff date; if the average technical performance and the average efficiency of T2 are above \( X^* \) and \(Eff^* \), T1 is prohibited. On the contrary, if T2 does not reach the targets, suppliers can keep on marketing T1 after the sunset date, but only if they prove that they carried out serious analyses of alternatives providing information on their R&D activity. In fact, suppliers with only T1 in their portfolio have to prove that they allocate a sufficient budget to the R&D watch on T2. Authorization is granted, and the supplier can keep on developing and marketing T1 until the next revision date only if the following condition is respected:

\[
RD_{\text{watch}}_{lt-1} \geq \alpha_{\text{Watch}} \times AvRD_{\text{watch}}{lt-1} \quad (18)
\]

with \( \alpha_{\text{Watch}} \) a parameter \( \in [0; 1] \) reflecting the severity of the regulation and \( AvRD_{\text{watch}} \) the average R&D watch performed in the industry. If this condition is not fulfilled, authorization is not granted and T1 is forbidden for the considered supplier. At the revision date, a similar sequential checking is made. The revision date is defined by adding the parameter \( \Delta T_{\text{revision}} \) to the sunset date.

Because the authorization process of regulation puts pressure on suppliers to develop and market T2, it will affect their decisions regarding innovation and production. Concerning innovation activities, with REACH the share of the global R&D budget affected by T1 is now defined as

\[
\delta_{T1} \times \left(1 - PS_{S} \times \frac{t}{T} \right)
\]

with \( PS_{S} \) a parameter \( \in [0; 1] \) reflecting the perceived stringency of regulation by suppliers\(^24\) and \( T \) alternatively the sunset date or the revision date. In terms of production activities, the adoption index used by supplier \( i \) to examine the possibility of introducing T2 into the market is now defined as follows:

\[
AdIndex_{lt}^{T2} = (K_{lt} + M_{lt}^{T2}) \times \left(1 + PS_{S} \times \frac{t}{T} \right) \quad (1')
\]

According to these changes, the higher the perceived stringency of regulation by suppliers and the closer the sunset or revision date is, the more they consider a T1 ban to be an actual threat, the more they will be induced to reorient their R&D activities toward T2, and the faster they will adopt and develop T2.\(^25\)

As to the extended producer responsibility, the aim is to get actors in the whole production chain to take into account the environmental and health impacts of the activity and to change the demand of downstream users toward safer substances. REACH extends the responsibility principle so that the technology portfolio held by suppliers matters in the clients’ decisions. First, the three-step purchase procedure is affected. The score functions \( (U) \) given to the product of suppliers holding a portfolio without T2 are weighted by a factor \( \left(1 - PS_{C} \times \frac{t'}{T} \right) \) with \( PS_{C} \) a parameter \( \in [0; 1] \) reflecting the perceived stringency of regulation by clients.\(^26\) Second, the two-step decision procedure made by a client to keep the same supplier or to switch to another supplier is now preceded by a prior step for clients whose supplier does not have T2 in its portfolio. This prior step consists of leaving the supplier with a probability given by:

\(^{24}\) The higher the \( PS_{S} \) is, the more suppliers perceive T1 ban as a credible threat.

\(^{25}\) This intuition is supported by empirical evidence showing that some firms are redirecting their R&D efforts under the REACH influence (CSES, 2012).

\(^{26}\) The higher the \( PS_{C} \), is, the more clients perceive the T1 ban to be a credible threat.
According to these changes, the higher the perceived stringency of regulation by clients and the closer the sunset or revision date is, the more they consider a T1 ban to be an actual threat, the more they will select and keep a supplier with T2 in its portfolio.

The model is now set up to represent and analyze (1) the role of objective and perceived stringency of the authorization procedure of REACH in cases when this procedure would apply to bisphenols; (2) the divergence of perception between suppliers and clients and thus the ensuing perception misfits; and (3) how these aspects influence dynamically the substitution of harmful substances.

4. Results

4.1. Experimental setup

We used the Laboratory for Simulation Development to compute and run the model.27 At the start of a simulation run, there were 10 suppliers and 200 clients. We ran 500 batches of simulations in order to cope with stochasticity and to generate different stories in order to hold out general propositions about the simulated industrial dynamics. We ran simulations with 250 time periods each in order to allow sufficient time for evolutionary processes to be implemented.28

We exhibit the main characteristics of industrial dynamics by considering the following indicators:

- The inverse Herfindahl-Hirshman index of concentration (1/HHI) is used to measure market concentration. The higher the 1/HHI is, the higher the degree of competition, and inversely.
- The cumulated number of exiting and entering suppliers29
- The market share of T2
- The global toxicity of the materials bought by clients (ToxAcc). This is a global indicator of the health risk of endocrine disruptors associated with the hazard properties of substances incorporated into the materials in use. In order to consider past accumulation of the toxic source and thus likely irreversible impacts even if exposition has ceased, we use the following equation:

\[ \text{ToxAcc}_t = \text{ToxAcc}_{t-1} + \sum_{j=1}^{M} \text{Tox}_{k,j,t} \]  

\( \text{Tox}_{k,j,t} \) is the toxicity level of the material \( k \) (T1 or T2) used by customer \( j \). The lower the \( \text{Tox} \) is, the lower the rhythm of additional toxicity. Such an indicator can only exhibit a growing trend if toxicity increases or a stabilization if toxicity ceases, thus creating a threshold below which it is not possible to go even if the pollution source has been removed.
- A global environmental indicator (BioAcc) that traces back the accumulation of substances in the environment defined by the following equation:

\[ \text{BioAcc}_t = \text{BioAcc}_{t-1} + \sum_{j=1}^{M} \text{Bio}_{k,j,t} \]

27 Laboratory for Simulation Development is a simulation platform developed by Valente (2008). It is downloadable at the following address: www.labsimdev.org. The programming file of the model is available on request.

28 We study the simulations outcomes by calculating every 25 time periods the average value of each indicator over the 500 simulations.

29 Three main causes of exit can occur: (1) lack of budget; (2) R&D watch on T2 lower than the required level, reflecting insufficient research on new alternative substances; (3) ban of T1, which forces firms with only T1 in its portfolio to exit.
\[
\text{BioAcc}_t = \text{BioAcc}_{t-1} - \text{ABS} + \sum_{j=1}^{M} \text{Bio}_{k,j,t}
\]  (21)

where \(ABS\) stands for the assimilative capacity of the ecosystem receiving hazardous substances during each period. It reflects the ability of the ecosystem to receive a determined level of residues, to degrade them, and to convert them in non-damaging substances (Pearce & Turner, 1990).\(^30\) \(\text{Bio}_{k,j,t}\) is the environmental risk of bioaccumulation of the material \(k\) (T1 or T2) used by customer \(j\). According to equation (21), the current accumulation of substances in the environment depends on its previous level minus assimilated residues by the ecosystem plus the current flow of hazardous substances.

Regarding parameter setting (see Appendix A), three sets of parameters are considered: empirically based parameters, technical parameters, and empirically uncertain parameters (Filatova et al., 2013). Parameters related to product characteristics\(^31\) are empirically based. Their maximum limit and their initial value are based on data to account for the difference in order of magnitude between bisphenol-based materials and bio-based substitution materials. Technical parameters are scale parameters that have been set to calibrate the model plausibly. Empirically uncertain parameters are randomly chosen in an admissible range because they are believed to have a particularly significant influence on the model outputs. A sensitivity analysis of this latter set of parameters has been performed in order to validate the model (see Appendix B).

4.2. The impact of regulation on technology substitution

In this section we first analyze the impact of objective stringency on technology substitution; we then study how these results are affected by a change in a subjective stringency of firms.\(^32\)

4.2.1. The role of objective stringency

Authorization and EPR are visible signs of public commitments toward technology substitution. Their implementation may then be more or less severe depending on the required level of techno-economic performance that substitutes must reach to replace existing substances and the time frame given to manage regulatory compliance. These levers of action actually apply to every firm in the chemical industry, thus displaying signs of “objectively” stringent measures.

We compare two opposite scenarios depending on the degree of severity in terms of target thresholds (required techno-economic performance and R&D watch) and on the timing of regulation (Table 1). The low objective stringency scenario combines soft targets and late timing whereas the high objective stringency scenario combines tight targets and early timing. The perceived stringency parameters (\(PS_C\) and \(PS_S\)) are set randomly between 0 and 1 such that the assessments by clients and suppliers extend along a continuum between perfectly credible and perfectly incredible. These two scenarios are compared with a benchmark situation without regulation.

\(^{30}\) \(ABS\) is set exogenous and constant over time.
\(^{31}\) Technical quality, productive efficiency, health risk of endocrine disruptors, and environmental risk of bioaccumulation are the characteristics used.
\(^{32}\) The sensitivity of the model to regulation parameters has been tested with a Monte Carlo procedure in order to confirm the findings presented in this section and to give them more robustness. The results of the sensitivity analysis are displayed in Appendix B.
Table 1. Policy variables and parameters for target thresholds and timing

<table>
<thead>
<tr>
<th>Target Thresholds</th>
<th>Techno-economic performances</th>
<th>R&amp;D watch</th>
<th>Timing</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>X* Cost* 𝛼_Watch</td>
<td>Sunset date</td>
<td>Revision date</td>
</tr>
<tr>
<td>Low objective stringency</td>
<td>High (9.3) Low (83.7) Low (0.1)</td>
<td>Late</td>
<td>Rare</td>
</tr>
<tr>
<td>𝛼_Watch</td>
<td>0.1</td>
<td>T_sunset=180</td>
<td>ΔT_revision=20</td>
</tr>
<tr>
<td>High objective stringency</td>
<td>Low (3.7) High (97.3) High (0.9)</td>
<td>Early</td>
<td>Frequent</td>
</tr>
<tr>
<td>𝛼_Watch</td>
<td>0.9</td>
<td>T_sunset=25</td>
<td>ΔT_revision=5</td>
</tr>
</tbody>
</table>

Quite similar overall results to Arfaoui et al. (2014) are observed (Figure 1). Only the most stringent scenario enables domination of T2 because of an early ban of T1, whereas the less stringent scenario is characterized by the coexistence of T1 and T2 but still in great favor of T1. Thus technology substitution from T1 to T2 does happen when regulation is very stringent, resulting in a significant reduction of environmental and health impact in the form of a reduction of the bioaccumulation stock and a stabilization of global toxicity near a relatively low threshold.

Figure 1. Evolution of the main indicators (average for 500 simulations)
In the high stringency scenario, the effective ban of T1 (about period 34 on average; see Table 2) goes with a great number of failures in the industry but only in a first place. Indeed every firm that still has T1 in its portfolio cannot use the technology anymore after the cutoff date. We observe then quick failures at the turning point for suppliers with only T1 in their portfolio. In turn, green pioneers specializing in T2 are rewarded with their risky attitude and can go on capitalizing on the green technology. Progress on T2 is thus early and rapid. Moreover, the radical selection of T2 resulting from the early ban of T1 brings a reduction in the market size (lower demand) because of unsatisfied demand regarding the new technology, which turns to be expensive and of low quality at the cutoff moment. Again the reduction in the market size contributes to an increase in firms’ exit and thus in the number of failures. In total, industry concentration increases and distribution of market shares appears significantly unbalanced. Entry is blocked because of higher entry barriers. However, after the significant shake-out brought out by the ban of T1, we observe a decrease of concentration because of renewed emulation among T2 suppliers leading to a stabilization of the industry around an oligopoly. In total, the high stringency scenario is characterized by a lower cumulated number of entries so that in the last period (t=250) the cumulated number of failures turns out to be lower than the one observed in the low stringency scenario. This result differs from the one found in Arfaoui et al. (2014) because of the entry process and endogenous mark-up rates. The strong selective pressure operated by regulation with the ban of T1 results in the survival of few firms able to share the market rather equally with relatively high mark-up rates and good profit levels, reducing opportunities for new entrants and enabling a rapid exploitation of technological opportunities offered by the potential of T2.

Table 2. Main indicators at time \( t=250 \) in the different scenarios

<table>
<thead>
<tr>
<th>Time ( t=250 )</th>
<th>Benchmark</th>
<th>High Objective Stringency</th>
<th>Low Objective Stringency</th>
</tr>
</thead>
<tbody>
<tr>
<td>T2 market share</td>
<td>11.91%</td>
<td>100% (<em><strong>), 61.7% (</strong></em>),</td>
<td></td>
</tr>
<tr>
<td>Inverse HHI</td>
<td>11.53</td>
<td>4.2 (***)</td>
<td></td>
</tr>
<tr>
<td>Bioaccumulation</td>
<td>124,263.11</td>
<td>0 (***)</td>
<td></td>
</tr>
<tr>
<td>Toxicity</td>
<td>232,941.02</td>
<td>84,752 (***)</td>
<td></td>
</tr>
<tr>
<td>Average cumulated number of failures</td>
<td>11.6</td>
<td>11.5 (***)</td>
<td></td>
</tr>
<tr>
<td>Average number of competitors</td>
<td>12.6</td>
<td>4 (***)</td>
<td></td>
</tr>
<tr>
<td>Number of customers</td>
<td>200</td>
<td>195</td>
<td></td>
</tr>
<tr>
<td>Minimum number of customers</td>
<td>196</td>
<td>57</td>
<td></td>
</tr>
<tr>
<td>Average mark-up T2</td>
<td>0.77</td>
<td>0.88 (***), 0.74 (n.s.)</td>
<td></td>
</tr>
<tr>
<td>Average mark-up T1</td>
<td>0.64</td>
<td>1.02 (***)</td>
<td></td>
</tr>
<tr>
<td>Time of T1 ban</td>
<td>-</td>
<td>34</td>
<td></td>
</tr>
<tr>
<td>Time of first T2 adoption</td>
<td>36</td>
<td>16</td>
<td></td>
</tr>
</tbody>
</table>

When regulation is soft (low stringency scenario), T1 is never prohibited, and firms specialized in T1 maintain a permanent advantage compared with firms having T2 in their portfolio even if they are disturbed by a regulatory threat during the whole time period. This situation explains why the reduction of the bioaccumulation stock is slow to come and materialize whereas the global toxicity only gradually slows down and ends up not so far from the final level obtained in the benchmark. In fact, similar to Arfaoui et al. (2014), regulation fails to promote technology transition from T1 to T2 because the blade never falls leaving clients with the possibility of purchasing T1 until the end and benefiting from the continuous improvements made to T1 to the detriment of T2, for which progress is small and continuously delayed. The failure to ban T1

A t-test has been carried out to check for significantly statistical differences between values for the benchmark and the high stringency scenario on the one hand and between the benchmark and the low stringency scenario on the other hand. (**) and (****) represent significant \( p \)-value at the 5% and 1% respectively. (n.s.) stands for “not significant.”
because of lenient performance targets and late timing inhibits further development of T2. Thus firms with T1 never experience a decrease in market size even though they are subject to a permanent check on their R&D watch and through this monitoring tool may be forced to exit the market. This situation continues with a continuous process of entry over the whole time period and the global result is a significant cumulated number of failures and a rather low market concentration.

4.2.2. The role of perceived stringency of the policy framework

We now examine the role of the perceived stringency parameters for clients and suppliers (PS\textsubscript{C} and PS\textsubscript{S}) in the high and low objective stringency scenarios studied in Section 4.2.1. For each scenario, we study four cases depending on the degree of stringency perceived by suppliers or clients\textsuperscript{34} (see Table 3).

<table>
<thead>
<tr>
<th>Low perceived stringency by suppliers</th>
<th>High perceived stringency by suppliers</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low PS\textsubscript{S} - Low PS\textsubscript{C} (PS\textsubscript{S} = 0.1; PS\textsubscript{C} = 0.1)</td>
<td>High PS\textsubscript{S} - Low PS\textsubscript{C} (PS\textsubscript{S} = 0.9; PS\textsubscript{C} = 0.1)</td>
</tr>
<tr>
<td>Low PS\textsubscript{S} - High PS\textsubscript{C} (PS\textsubscript{S} = 0.1; PS\textsubscript{C} = 0.9)</td>
<td>High PS\textsubscript{S} - High PS\textsubscript{C} (PS\textsubscript{S} = 0.9; PS\textsubscript{C} = 0.9)</td>
</tr>
</tbody>
</table>

Results show that perceived stringencies have a weak impact on the high objective stringency scenario: objective stringency is self-sufficient to stimulate technology transition. Perceptions of suppliers and clients barely matter. The effect is to speed up the transition process from the moment when the blade has fallen (Figure 2). In that case the effective ban of T1 leads to select a de facto standard for T2. Every firm is carrying R&D activities on T2, every client has no choice but to buy T2, and continuous progress occurs until technological opportunities on T2 are exhausted.

Figure 2. Evolution of the T2 market share in the high objective stringency scenario (average for 500 simulations)

\textsuperscript{34} As a reminder, perceived stringency on the supply side plays when firms have to decide whether to adopt or not the new technology T2. Higher perception gives more weight to the timing of regulation, thus inducing the firm to adopt T2 more rapidly. Perceived stringency also plays in the allocation of R&D. Higher perception induces the firm to redirect its R&D efforts toward T2, through either the R&D watch budget or the R&D budget once T2 has been adopted. On the client side, perceived stringency also plays at two places: purchase and product replacement. Higher perception induces clients to less-valued products coming from suppliers with a portfolio exclusively dedicated to T1. This influence operates when a client has to decide which product to buy and when the client has to decide whether to keep or leave the current supplier.
Having said that, perceived stringency by suppliers and clients turns out to have a relatively stronger impact on the diffusion speed of the technology for T2. The first adoption of T2 and its diffusion in the industry are accelerated when stakeholders perceive the T1 ban to be a credible threat. The regulatory targets are reached faster putting into effect the sanction of prohibiting T1. The early diffusion of T2 leads to an early radical decrease in environmental and health negative effects. However, the influence of divergent perception between suppliers and clients only matters during the first stage of industrial dynamics because the intense and relatively quick turbulence phase first experienced by the industry is followed in every case by a phase of stabilization around an oligopoly.

More interestingly, perception happens to matter in the low objective stringency scenario (Figure 3). All things being equal, we observe that perceived stringency by clients has a significant positive impact on the T2 market share and on industry concentration: the higher clients perceive the regulatory threat is, the higher the diffusion of T2 ($M_{T2} > 70\%$) and the lower the number of suppliers at the end of the simulation period (Table 4). Environmental and health performances are also significantly improved. In that case, clients transmit their strong beliefs in the regulatory threat by giving preference to T2-based products, thus inducing suppliers to increase their innovative efforts on T2 and to adopt T2 without necessarily abandoning T1. This demand-pull effect favors suppliers with a mixed portfolio and green pioneers so that competition is fiercer between those firms and concentration increases. Though late (about period 226 on average), regulatory enforcement by way of the effective T1 ban is again made possible because of the cumulative improvements achieved on T2 stimulated by the high perceived stringency of regulation by clients. In the end, in the low objective stringency scenario, results are always better when the perceived stringency of regulation by clients is high whatever the perception of suppliers, and a positive link is found between perceived stringency by clients and environmental and health performances.
Perceived stringency of regulation by suppliers plays an ambiguous role. When perceived stringency by suppliers is high, T2 diffuses more, but unexpectedly it brings bad environmental and health performances. Actually, if perceived stringency by clients is low, we observe that T2 market share is higher when perceived stringency by suppliers is high than when it is low (see Table 4): 40% versus 21% at time $t=250$, as well when perceived stringency by clients is high: 87% versus 71% at $t=250$. However, regarding global toxicity, if perceived stringency by clients is low, we observe that that indicator exhibits a lower performance when perceived stringency by suppliers is high than when it is low: 269,989 versus 235,292 at time $t=250$ (the lower the better), as well when perceived stringency by clients is high: 186,416 versus 159,962 at $t=250$. Concerning the bioaccumulation indicator the difference is less marked when client perception is already high but is still valid in the opposite case. This result suggests that, in a low objective stringency scenario, it is desirable that suppliers weakly perceive the regulatory threat. Such a counterintuitive result is explained as follows: when perceived stringency by suppliers is high, they reorient their R&D watch or their R&D budget toward T2 and they adopt it more rapidly, thus also being more likely to neglect the improvement of the conventional technology T1; the contradiction is that technology T1 is almost never prohibited in that scenario, and clients go on

Table 4. Main indicators at time $t=250$ in the low objective stringency scenario

<table>
<thead>
<tr>
<th>Values at Time $t=250$</th>
<th>High $P_{S}$ - High $P_{C}$</th>
<th>High $P_{S}$ - Low $P_{C}$</th>
<th>Low $P_{S}$ - High $P_{C}$</th>
<th>Low $P_{S}$ - Low $P_{C}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>T2 market share</td>
<td>87.4%</td>
<td>39.95%</td>
<td>71.7% (***)</td>
<td>21.52% (***)</td>
</tr>
<tr>
<td>Inverse HHI</td>
<td>7.52</td>
<td>11.3</td>
<td>6.01 (***)</td>
<td>10.43 (***)</td>
</tr>
<tr>
<td>Bioaccumulation</td>
<td>25,345.87</td>
<td>121,972.86</td>
<td>27,730.55 (n.s.)</td>
<td>118,420.15 (**)</td>
</tr>
<tr>
<td>Toxicity</td>
<td>186,416.27</td>
<td>269,989.73</td>
<td>159,962.48 (***)</td>
<td>235,292.44 (***)</td>
</tr>
<tr>
<td>Average cumulated number of failures</td>
<td>13.5</td>
<td>13.2</td>
<td>14.1 (***)</td>
<td>11.7 (***)</td>
</tr>
<tr>
<td>Average cumulated number of entrants</td>
<td>12.2</td>
<td>15.8</td>
<td>11.2 (***)</td>
<td>13.9 (***</td>
</tr>
<tr>
<td>Average number of competitors</td>
<td>8.8</td>
<td>12.7</td>
<td>7.1 (***)</td>
<td>12.3 (***</td>
</tr>
<tr>
<td>Number of customers</td>
<td>200</td>
<td>200</td>
<td>200</td>
<td>200</td>
</tr>
<tr>
<td>Minimum number of customers</td>
<td>194</td>
<td>196</td>
<td>194</td>
<td>196</td>
</tr>
<tr>
<td>Average mark-up T2</td>
<td>0.72</td>
<td>0.67</td>
<td>0.84 (***)</td>
<td>0.76 (***</td>
</tr>
<tr>
<td>Average mark-up T1</td>
<td>0.68</td>
<td>0.65</td>
<td>0.74 (***)</td>
<td>0.64 (n.s.)</td>
</tr>
<tr>
<td>Time of T1 ban</td>
<td>226</td>
<td>227</td>
<td>34</td>
<td>37</td>
</tr>
<tr>
<td>Time of first T2 adoption</td>
<td>25</td>
<td>25</td>
<td>34</td>
<td>37</td>
</tr>
</tbody>
</table>

$35$ A $t$-test has been performed to check for significantly statistical differences between averages for high $P_{S}$ - high $P_{C}$ and low $P_{S}$ - high $P_{C}$ and between averages for high $P_{S}$ - low $P_{C}$ and low $P_{S}$ - low $P_{C}$. (*) $(**)$, and $(***)$ represent significant $p$-values at the 10%, 5%, and 1% respectively. (n.s.) stands for “not significant.”
buying T1, having low incentives to buy T2. As a consequence, environmental and health improvements achieved through T1, though incremental compared with the possibilities offered by T2, are less possible and fall short leading to almost unchanged environmental performances and worse health performances than those achieved in the benchmark (see Table 5).

Table 5. Environmental and health performances at time \( t=250 \) in different scenarios.\(^{36}\)

<table>
<thead>
<tr>
<th>Values at Time ( t=250 )</th>
<th>Benchmark</th>
<th>Low Objective Stringency</th>
<th>Low Objective Stringency</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>High ( P_{Yt} ) - Low ( P_{Yc} )</td>
<td>Low ( P_{Yt} ) - Low ( P_{Yc} )</td>
</tr>
<tr>
<td>Bioaccumulation</td>
<td>124,263</td>
<td>121,972 (n.s.)</td>
<td>118,420 (***))</td>
</tr>
<tr>
<td>Toxicity</td>
<td>232,941</td>
<td>269,989 (***))</td>
<td>235,292 (n.s.)</td>
</tr>
</tbody>
</table>

In that particular situation, environmental and health progress is achieved thanks to the wider adoption of T2, but it does not compensate the lower incremental advances on T1 in which R&D is forsaken because of the conjunction between strong beliefs in T2 by suppliers and soft regulation. In the end, looking at environmental and health performances in the low objective stringency scenario, results are better if there is consistency between supplier perception and objective stringency: both should be low together! Otherwise regulation is useless because environmental and health performances are either not improved or even worse compared to the configuration without regulation (benchmark).

5. Discussion

The ABM we propose to study policy impacts on substitution of bisphenols highlights three main outcomes. First, substitution of bisphenols calls for a significantly stringent regulation. This means that (1) the substance first must be subject to authorization for being used after the sunset date, (2) high techno-economic performance targets are used to scrutinize alternative substances, and (3) timing of the sunset and, if applicable, revision dates for granting authorization is tight. Having that in mind, it is clear that REACH is delaying the moment when bisphenols are prohibited, thus sending wrong signals about their effective ban and causing a gap between the technological risks taken by suppliers to develop alternative substances and what actually affects the regulatory process. This finding confirms that delay in intervention is costly: the sooner and stronger the policy response is, the shorter the slow growth transition phase (Acemoglu et al., 2012). We further show that the later and weaker the policy response is, the more inefficient and useless the regulation to support substitution.

Second, high objective stringency brings consequences to the market structure and entry barriers. We show that objectively high stringency results in a stable oligopoly after experiencing an early but short turbulent phase because of the ban of the dangerous substance. This phase is characterized by a significant reduction in demand, number of competitors, and number of available technologies. Subsequently, entry barriers are stronger and less entry is possible. In this regard opportunities to exploit the new cleaner technology are lower and established firms have good innovative performances as long as they are potentially challenged by new entrants. For regulators, environmental policy should go together with competition policy not in a rigid way but following a rule-of-reason approach. From the start, compliance with competition law as part of REACH-related activities has been a challenging issue (Béal et al., 2013; Béal & Deschamps, 2014; Fuchs, 2011; Scott & Trubek, 2002). Regulators should go beyond an opposition between environmental policy and competition policy. They should consider environmental policy designed to foster eco-innovation as affecting the market structure in such a way that higher industrial concentration resulting from a product ban is no more than the outcome of a selection process in favor of harmless substitutes and by which the conventional firms are forced to exit.

\(^{36}\) A \( t \)-test has been performed comparing values for each scenario against the benchmark. (***)) significant at 1%; (n.s.) not significant.
and the green firms can survive. Because we can expect higher concentration from strong policy stringency, a rule-of-reason approach would be needed to examine the necessary trade-offs among fast environmental and health benefits, temporary demand mismatches, and higher industrial concentration. In our model radical innovation is generated by incumbents, but they are subject to the permanent threat of entry of new firms inducing incumbents to increase R&D investments to preserve or enhance their market shares. Making market entry attractive to new players is thus also essential to favor radical innovation. This condition echoes the one underlying the complementarity hypothesis developed by Nesta et al. (2014) in which environmental policies are more effective in competitive markets.

Third, the way industrial actors perceive the regulatory threat may be important to consider when assessing technology transition. More specifically, perception matters only when regulation is soft. Indeed an objectively stringent regulation implies enough strict targets and early timing to be self-sufficient to promote technology substitution. In that case, the way agents perceive the regulatory threat only accelerates or slows down the transition. By contrast, in the case of a lenient regulation, it will be all the more efficient when suppliers perceive it soft but confront clients that sense it is severe: suppliers are induced to faster adopt and sell the new technology because of a strong demand pressure but they simultaneously keep on developing the old technology, which thus coexists with the new one. In the end, environmental and health performances are improved compared to the benchmark when perception misfits are strong between suppliers and users. More generally, perception of clients plays a major role in stimulating substitution when regulation severity is low, thus conveying a significant demand-pull effect. In terms of policy implications, labeling may be a crucial tool helping clients to better perceive the regulatory threat. In connection with REACH, labels give higher visibility to credence products characterized by attributes buyers cannot confidently evaluate, even after one or more purchases. As well, labels force defining criteria for the identification of substances with endocrine-disrupting properties. Thus it would make the subsequent classification of these substances under REACH easier, and by communicating their hazards it would make clients increasingly suspect their likely ban. Another way of reinforcing clients’ perception resides in the commitments of the main regulator ECHA, which should exhibit more consistency over time. Especially, present and future commitments regarding the authorization process should increase its credibility and legitimacy. Finally, innovation policy tools are also a means to increase the awareness of clients because it gives more credibility to the fact that new alternatives are searched for and might be techno-economically available in the near future. Demonstration projects, technology platforms, and subsidies are some of the tools able to support suppliers when changing their technology portfolio and at the same time strengthen clients in their beliefs of a tough policy stance.

6. Conclusion

In this article we developed an ABM aimed at investigating the authorization procedure of the REACH regulation in the case of bisphenol-based materials. Belonging to the community of ABM users we argue is a useful tool to analyze complex systems incorporating novelty and coevolution of heterogeneous behaviors and at the same time enables focusing on specific components such as policy design aspects. One main drawback comes from the use of sometimes ad hoc assumptions or very peculiar mechanisms of change. Yet we believe that our results are valid and robust insofar as the most relevant parameters are empirically based.

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37 As is the case with regulation (EC) 1272/2008 on the classification, labeling, and packaging of substances and mixtures (CLP), which introduces the United Nations globally harmonized system (UN GHS) for classification and labeling of chemicals into Europe.
robustness analysis is made with a Monte Carlo procedure, and results are confronted with empirical data as much as possible.

The ABM enabled operationalization of some aspects that matter to designing environmental policy to spur eco-innovation. In addition to high techno-economic levels of performance target and tight timing, objective stringency alone appears important but not always sufficient for warranting successful substitution. Our ABM shows that the extent to which the authorization procedure is effective may depend on policy stringency perception. Perceived stringency receives explicit attention in our model thus echoing – though modestly – the role of psychology of uncertain decisions blurred by contradictory messages from institutions (Brocas & Carrillo, 2004). In that perspective, regulation is a driver of change and a way to serve industrial interests, leaving room for interpretation and heterogeneous perception of the regulatory threat (Lascoumes, 1994). Our model shows the configurations in which perception is having an impact on global dynamics. In particular when objective stringency is weak, subjective stringency of suppliers matters but not in the expected way because high perceived stringency by suppliers brings no improved environmental performances and even lower health performances compared to those achieved without regulation or those obtained when perceived stringency by suppliers is low. Thus, in a context of soft objective stringency, it is preferable that suppliers perceive it as such and yet confront clients with a strong perception. This finding corroborates that perception misfits at the individual level are an important determinant of environmental and health performances at the industry level.

Our model is a second step toward a stylized framework that can be used to explore the dynamic interplay between environmental regulation and innovation. Further developments are suggested. First, what is called T2 in our formalization is far more heterogeneous than what is assumed in the first place: a multitude of substitutes in idiosyncrasy with specific uses should instead be studied. Second, it would be useful to consider different supplier strategies and thus diversified technology portfolios because of different geographical markets not subject to the same regulatory constraints (REACH in Europe versus chemicals policy in the United States, Japan, and China). Another line of future research would be to study the interplay among environmental, competition, and innovation policies. Various policy instruments could be studied: tax, subsidy, eco-patents, mix of instruments adapted to the phase of the technology life cycle in order to provoke synergy effects of policies supporting radically new technologies, and thus give policy makers the possibility to fine-tune the authorization procedure and fill the gap between the spirit and letter of REACH.
References


ChemSec, 2015. Authorization process needs further fine-tuning not to disfavor alternative producers. Note from the International Chemical Secretariat, March.


Appendix A. Overview of parameter setting and initialization of variables

Symbols by category of parameters (empirically based: ♠; technical: ♣; empirically uncertain: ♦)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial number of firms ♠</td>
<td>10</td>
</tr>
<tr>
<td>Number of clients ♠</td>
<td>200</td>
</tr>
<tr>
<td>Number of products ♠</td>
<td>Number of characteristics ♠</td>
</tr>
<tr>
<td>Potential for each product characteristic ♣</td>
<td></td>
</tr>
<tr>
<td>T1</td>
<td>Xmax, Effmax, Toxmin, Bioimin</td>
</tr>
<tr>
<td>T2</td>
<td>Xmax, Effmax, Toxmin, Bioimin</td>
</tr>
<tr>
<td>Initial values of each product characteristic ♣</td>
<td></td>
</tr>
<tr>
<td>T1</td>
<td>X0, Eff0, Tox0, Bio0</td>
</tr>
<tr>
<td>T2</td>
<td>X0, Eff0, Tox0, Bio0</td>
</tr>
<tr>
<td>Purchase decision</td>
<td></td>
</tr>
<tr>
<td>Client’s preferences: PrefX, PrefP, PrefTox, PrefBio ♦</td>
<td>[0; 1]</td>
</tr>
<tr>
<td>Parameters: ZX, ZP, ZTox, ZBio ♣</td>
<td>0; 1075; 20; 20</td>
</tr>
<tr>
<td>Bandwagon effect: z ♦</td>
<td>0.05</td>
</tr>
<tr>
<td>Reserve price ♦</td>
<td>[97; 715]</td>
</tr>
<tr>
<td>Minimum product quality ♦</td>
<td>[3; 9]</td>
</tr>
<tr>
<td>Rebuy decision</td>
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</tr>
<tr>
<td>Tolerance parameter Tol ♦</td>
<td>[0.8, 1.2]</td>
</tr>
<tr>
<td>Total budget</td>
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</tr>
<tr>
<td>Initial budget B0 ♣</td>
<td>1944</td>
</tr>
<tr>
<td>Fixed costs FC ♣</td>
<td>250</td>
</tr>
<tr>
<td>Initial mark-up rate ♣</td>
<td></td>
</tr>
<tr>
<td>T1</td>
<td>µ0</td>
</tr>
<tr>
<td>T2</td>
<td>µ0</td>
</tr>
<tr>
<td>Exit/entry</td>
<td></td>
</tr>
<tr>
<td>Maximum probability of entry αEntry ♦</td>
<td>0.1</td>
</tr>
<tr>
<td>Absorptive capacity ♦</td>
<td>[0.8; 1.2]</td>
</tr>
<tr>
<td>Production costs</td>
<td></td>
</tr>
<tr>
<td>Scale parameter αCost ♣</td>
<td>0.009</td>
</tr>
<tr>
<td>Parameters: AX, AEff, ATox, ABio ♣</td>
<td>0; 20; 20; 20</td>
</tr>
<tr>
<td>Technology portfolio</td>
<td></td>
</tr>
<tr>
<td>Decision to adopt T2</td>
<td></td>
</tr>
<tr>
<td>Adoption threshold ♦</td>
<td>[0; 2]</td>
</tr>
<tr>
<td>Initial switching costs ♣</td>
<td>1250</td>
</tr>
<tr>
<td>Decision to leave T1</td>
<td></td>
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<tr>
<td>Abandon threshold ♦</td>
<td>[0.5; 1]</td>
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<tr>
<td>Innovation process</td>
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<tr>
<td>Initial R&amp;D budget ♣</td>
<td>388.8</td>
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<tr>
<td>R&amp;D rate δ ♦</td>
<td>0.2</td>
</tr>
<tr>
<td>R&amp;D share allocated to T1 δT1 ♦</td>
<td>[0; 1]</td>
</tr>
<tr>
<td>Speed αI ♦</td>
<td>0.0015</td>
</tr>
<tr>
<td>Scale parameters βX, βEff, βTox, βBio ♣</td>
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</tr>
<tr>
<td>R&amp;D watch</td>
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</tr>
<tr>
<td>Speed αw ♦</td>
<td>0.0015</td>
</tr>
<tr>
<td>Knowledge accumulation</td>
<td>Scale parameter αK ♣</td>
</tr>
<tr>
<td>Kmax ♣</td>
<td>1</td>
</tr>
<tr>
<td>Switching costs</td>
<td>Scale parameter αs ♣</td>
</tr>
<tr>
<td>Smin ♣</td>
<td>625</td>
</tr>
<tr>
<td>Global indicator</td>
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<tr>
<td>Assimilative capacity of the ecosystem ABS ♣</td>
<td>940</td>
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</tbody>
</table>
Appendix B. Sensitivity analysis

We perform a sensitivity analysis of results to parameters based on a set of simulations carried out with a Monte Carlo procedure. By running a high number of simulations (10,000) with a random setting of the values of the parameters, this procedure generates a large number of possible outcomes covering a diversified subset of the parameter space. We perform a two-step sensitivity analysis. First, we test the validity of the model by investigating the benchmark situation without regulation. We focus on parameters we have considered to be empirically uncertain and to which the model is most highly sensitive. Second, we assess the sensitivity of the model to regulation parameters to give more robustness to the results presented in Section 4.2. The chosen domain of parameters in the Monte Carlo procedures is presented in Table B.1. We process results with regression trees. A regression tree (Venables & Ripley, 1999) establishes a hierarchy between independent variables using their contributions to the overall fit ($R^2$) of the regression. The tree gives a hierarchical sequence of conditions on the parameters of the model: the higher the role of a condition in the classification of the observed case is, the higher its status on the tree. For each condition, the left branch shows the cases for which the condition is true and the right branch indicates cases compatible with the complementary condition. The two numbers at the leaves of the trees are the expected value of the dependent variable and the number $n$ of observations for which the condition(s) on the parameter(s) is (are) satisfied. Dependent variables are the main indicators presented in Section 4.1 (market share of T2, inverse Herfindahl-Hirschman index of concentration, bioaccumulation, and toxicity indicator). Independent variables are the parameters presented in Table B.1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Purchase decision</strong></td>
<td></td>
</tr>
<tr>
<td>Average value for client’s preferences $Av_{PrefX}$, $Av_{PrefP}$, $Av_{PrefTox}$, $Av_{PrefBio}$</td>
<td>$[0; 1]$</td>
</tr>
<tr>
<td>Bandwagon effect $z$</td>
<td>$[0; 0.1]$</td>
</tr>
<tr>
<td>Average value for reserve price $Av_{resP}$</td>
<td>$[97; 715]$</td>
</tr>
<tr>
<td>Average value for minimum product quality $Av_{minX}$</td>
<td>$[3; 9]$</td>
</tr>
<tr>
<td><strong>Total budget</strong></td>
<td></td>
</tr>
<tr>
<td>Fixed costs $FC$</td>
<td>$[125; 375]$</td>
</tr>
<tr>
<td><strong>Exit/entry</strong></td>
<td></td>
</tr>
<tr>
<td>Maximum probability of entry $\alpha_{in}$</td>
<td>$[0; 0.2]$</td>
</tr>
<tr>
<td>Average value for absorptive capacity $Av_{abso}$</td>
<td>$[0.8; 1.2]$</td>
</tr>
<tr>
<td><strong>Technology portfolio</strong></td>
<td></td>
</tr>
<tr>
<td>Decision to adopt T2</td>
<td>$[0; 2]$</td>
</tr>
<tr>
<td>Decision to leave T1</td>
<td>$[0.5; 1]$</td>
</tr>
<tr>
<td><strong>Innovation process</strong></td>
<td></td>
</tr>
</tbody>
</table>

38 For instance considering Figure B.1, on the left branch of the tree, we have all observations for which $\alpha < 0.00141$. On the right branch, we have all observations for which $\alpha \geq 0.00141$. When $\alpha \geq 0.00141$ and $\alpha < 0.001263$, the expected value for the market share of T2 is 7.224%, and we have $n = 2204$ observations (over 10,000) corresponding to this case.

39 Firm-specific and consumer-specific parameters are chosen so that their average value over the population is within the admissible range presented in the table.
Regarding the benchmark situation, Figures B.1 to B.4 show that parameters of R&D activities and innovation have a crucial impact on the model dynamics. The higher the proportion (\( \delta \)) of the budget of firms allocated to R&D activities, the higher the market concentration (Figure B.2) because the remaining budget will tend to be lower, which increases the risk of bankruptcy. This combination of high investment in R&D and high market concentration will enable firms to lower faster pollution and toxicity of their products (Figures B.3 and B.4). Pollution and toxicity are all the more reduced because of the larger diffusion of T2, actually, when the speed of the innovation process (\( \alpha_i \)) is high (Figures B.1, B.3, and B.4).40 The market share of T2 (Figure B.1) also depends positively on the speed at which the level of the current R&D expenditure enables knowledge accumulation (\( \alpha_w \)), and negatively on the share of total R&D allocated to T1 (\( \delta_{T1} \)) and the average value for adoption threshold (\( Av_{\text{adopt}} \)). In fact, the combination of fast accumulation of knowledge, large investment in technological watch on T2, and fast market introduction of T2 would enable faster progress in the performance of T2, making this technology quickly attractive. Finally, Figure B.2 shows that large fixed costs tend to increase market concentration because they increase the probability of failure, and by limiting the number of competitors low probability of entry also increases market concentration.

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40 One can notice that when technological change is slow, concentration is low (Figure B.2). In that case, there is very little opportunity to differentiate products thanks to innovation. This situation leads to a homogenous distribution of firms’ market shares and persistent competition.
Figure B.1. Regression tree of T2's market share (benchmark)

Figure B.2. Regression tree of inverse HHI (benchmark)

Figure B.3. Regression tree of bioaccumulation indicator (benchmark)
As to the sensitivity of the model to regulation parameters, trees confirm our finding that regulation outcomes depend dramatically on objective and perceived stringencies. High objective stringency is reflected on trees by low techno-economic performance targets $X^*$ and $Eff^*$ and early sunset date $T_{sunset}$. Figure B.5 shows that high objective stringency enables domination of T2 because of an early ban of T1. It results in a significant reduction of environmental and health impacts (Figures B.7 and B.8) and a significant increase in market concentration (Figure B.6) because of a great number of failures in the industry and unbalanced market shares. The same outcomes are obtained with high perceived stringency of regulation by clients reflected by high value for $PS_C$. Thus, Figure B.5 shows that the largest diffusion of T2 (94.61% market share) is observed when the performance target $X^*$ is strict ($X^*<7.066$) and clients perceive the regulation to be stringent ($PS_C≥0.2208$). Contrary to $PS_C$, the parameter $PS_S$ does not appear on any tree confirming that perceived stringency of regulation by suppliers plays only a secondary role in the dynamics.
Figure B.7. Regression tree of bioaccumulation indicator (regulation)

Figure B.8. Regression tree of toxicity indicator (regulation)
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