Policy Design, Eco-innovation and Industrial Dynamics in an Agent-Based Model

An Illustration with the REACH Regulation

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Abstract: The paper proposes an agent-based model to study the impact of European regulation REACH on industrial dynamics. This new regulation adopted in 2007 establishes a new philosophy in how to design environmental protection and health. For this reason, REACH appears as a privileged object of study to analyze the impact of regulation on innovation strategies of firms and the market structure. Our model focuses on the interactions between clients and suppliers in order to take into account interdependencies at the heart of vertical relationships that are upset by the new principles introduced by REACH. The main contribution of this paper is to show, through an agent-based model, how different combinations of flexible and stringent instruments designed on REACH regulation (Extended Producer Responsibility, authorization process and restrictions) create the incentives and the constraints to shape market selection and innovation.

1 INTRODUCTION

In 2006, after a long ‘legislative battle', the European Union (EU) adopted the REACH Regulation (Registration, Evaluation and Authorization of Chemicals) one of the most ambitious stringent regulation. This regulation introduces a new legislative philosophy in how to handle chemicals. Firstly, REACH adopts the “*principle of reversal of the burden of proof*” from authorities to industry. This principle postulates that manufacturers and importers of chemicals must register each substance used in a quantity higher than one tone per year, and assess the health and environmental risks associated; otherwise they will be automatically excluded from the market ("No data, no market"). Secondly, REACH extends responsibility also to users, since they are now responsible for the compliance of their production factors to the requirements of the new regulation. The downstream user is closely associated with regulatory compliance, by actively supporting the efforts of producers of substances. REACH does not apply only to the chemical industry but concerns all the industries. Lastly, a revolutionary aspect of chemicals regulation under REACH lies in a process of authorization and restriction to the most dangerous substances. Public authorization is required for the production and use of chemicals considered to be especially worrisome: so-called substances of very high concern (SVHC) "with the aim of substituting them". SVHC are to be gradually identified and once included in the Annex, they cannot be placed on the market or used after a date to be set (the so-called "sunset date") unless the company is granted an authorization. All request of authorization must be accompanied by a safety report and an analysis of alternatives. Thus, with the REACH Regulation, the precautionary principle is complemented by a substitution principle.

From the start, REACH has been designed to balance environmental objectives with competitiveness aims, and has the scope to induce the development and adoption of eco-innovation as a side-effect of the regulation itself. Eco-innovation can be defined as “the production, assimilation or exploitation of a product, production process, service or management or business methods that is novel to the organization (developing or adopting it) and which results, throughout its life cycle, in a reduction of environmental risk, pollution and other negative impacts of resources use (including energy

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use) compared to relevant alternatives" (MEI Report, 2007). In the economic literature, many authors have emphasized a positive correlation between innovation and environmental regulation (cf. EEA, 2011, for an overview). However, eco-innovations cannot be considered to be a systematic response to regulation. Policy design turns to be essential in inducing the development of eco-innovations (Ashford et al., 1985); (Hahn, 1989); (Johnstone, 2007); (Jänicke, 2008). In this respect, a number of criteria such as stringency, flexibility, timing and credibility are important factors to consider. REACH seems to fit perfectly in this context and appears as a privileged object of study to analyze how policy design can stimulate or allow eco-innovation.

This paper tries to model the key principles and mechanisms on which REACH relies on in an agent-based model. We try to show how different combinations of flexible and stringent instruments designed on REACH regulation (such as derived from the Extended Producer Responsibility principle and from the approval process and restrictions) create the incentives and the constraints to shape market selection and innovation. In particular, the model is intended to assess in which extent increased obligations on SVHC through authorization provisions may lead to increased moves towards the substitution of those substances through the supply chain.

The paper is organized as follows. Section 2 draws on the literature on eco-innovation to underline the importance of policy design in inducing the development of eco-innovation. In this perspective, we bring into light the main mechanisms of the REACH regulation that can stimulate innovation and substitution of chemical substances. Section 3 presents the model following the ODD (Overview, Design concepts, Details) protocol (Grimm et al., 2006), (Grimm et al., 2010). Such a protocol provides a standard procedure for describing Agent-Based Models (ABMs) in order to make them easier to analyze, understand and communicate. Section 4 presents the baseline simulations and examines the impact of regulation upon the market dynamics by considering various configurations in the policy design, especially through the flexibility and the stringency variables. Section 5 concludes.

2 ENVIRONMENTAL REGULATION AND INNOVATION

Theoretical and empirical analyses on the relationship between environmental regulation and innovation agree that eco-innovations are essentially "policy-driven" (Jänicke, 2008). Policy design turns to be essential, especially to spur eco-innovation.

2.1 Policy Design

We know from Porter and van der Linde (1995) that « *properly designed environmental standards can trigger innovation that may partially or more than offset the costs of complying with them* » in some instances (p.98). Porter argues that more stringent environmental policies will lead to innovations to reduce inefficiencies, and this, in turn, will eventually reduce costs. This process may take some time. Thus, only well-designed regulations lead to innovation. In particular flexible regulatory policies give firms greater incentives to innovate and thus are better than prescriptive forms of regulation. In many instances, these innovations are likely to more than offset the cost of regulation.

According to Ashford et al. (1985) and Hahn (1989), regulators must be careful to the severity, the flexibility and the timing of the regulation. Policy design is essential in inducing the development of eco-innovations (Jänicke, 2008). The policy design should in particular be based on ambitious and reliable targets; and provide a flexible policy mix supporting the innovation process from invention to diffusion.

In the way REACH has been designed, the European Commission was very attentive to these criteria. A combination of hard and soft law has been preferred such that REACH relies more on open-ended standards (Fuchs, 2011) that combine different criteria: stringent, reachable and flexible. As a matter of fact, the consequences of an incorrect application of the REACH Regulation are serious and immediate as they result in exclusion from market "No data, no market". Moreover, Fuchs (2011) describes REACH as a pragmatic regulation which is both ambitious and realistic in his goals in order to represent real incentive to undertake innovation. Pragmatism lies also in other provisions such as the multiple deadlines for phase-in substances, the collective setting of priorities under the authorization and restriction processes, the various exemptions incorporated in the regulation, or the limited risk assessment requirements for substances placed on the market in proportions of less than 10 tones. Lastly, flexibility is present through open-ended standards, flexible and revisable guidelines, and other forms of “soft law”. It was important that the system remain flexible in order to ensure its workability (Fuchs, 2011). Moreover, REACH promotes a mode of governance based on the idea of "self-responsibility". This approach involves giving more responsibilities to companies and more flexibility on how to achieve the goals (Fuchs, 2011). In total, these mechanisms can adapt to diversity, tolerate alternative approaches to problem-solving, and make it easier to revise strategies and standards in light of evolving knowledge (Scott and Trubek, 2002).

2.2 The Effect of REACH on Innovation

REACH has been designed to enhance innovation. For Nordbeck and Faust (2003), innovation is "the most important advantage of the REACH regulation". It is possible to modify the technological trajectory in the chemical industry and increase innovation towards sustainable development. According to Eurostat (2009), a number of innovation-friendly mechanisms in the chemical industry are present in REACH. In our model, we mainly focus on two crucial mechanisms that can promote innovation in the chemical industry: the authorization process and the extended responsibility principle.

The authorization procedure for substances of very high concern is connected to the principle of substitution. The purpose of the authorization is to ensure that the risks from substances of very high concern are properly controlled and that these substances are progressively replaced by other substances or technologies where these are economically and technically viable. The authorization procedure is based on several steps: identification of substances; request for authorization before the sunset date; granting or refusing authorization; review of authorization.

Substances eligible for authorization are identified by a Member State or the European Commission and are included in a list of substances of concern “substances of very high concern” (SVHC) listed in Annex XIV. Once included in that Annex, every firm willing to use such a substance must request for authorization before the “**sunset date**”. Thus, SVHC cannot be placed on the market or used after the “sunset date” unless the company is granted an authorization.

The granting or refusal of authorization is primarily based on the existence of economically and technically viable alternatives. So, in the event that there are economically viable alternatives, companies will no longer be allowed to use substances after the sunset date. However if there are no technically and economically viable alternatives, authorizations are granted *only if* firms prove that they carry out serious analyses of alternatives. In fact, under Article 5 of the regulation, all request of authorization must be accompanied by a safety report and an analysis of alternatives with information about activities of Research and Development (R&D). In that case, authorizations are granted until a specific date by which the holder of the authorization will have to resubmit an application. **Review dates** are set on a case by case basis and are driven by the information provided by the applicant, in particular the substitution plan and the analysis of alternatives. To renew an authorization, a revised report must be sent to ECHA (the European Chemicals Agency) before the expiry date of **the time-limited review period** defined in the authorization decision. Meanwhile, the authorization may be reviewed or suspended by the Commission *at any time*, if information regarding possible replacement substances becomes available or the circumstances of the authorization have changed. So firms are encouraged to maintain technology watch on alternatives. We see that the process of authorization is characterized by different time variables that combine stringency (the sunset date) and flexibility (review date), but also pragmatism (cost-benefit analysis) in order to support the innovation process from invention to diffusion.

The second innovation-friendly mechanism present in REACH lies in the **extended responsibility to users** since they are now responsible for the compliance of their factors of production to the requirements of the new regulation. According to Wolf and Delgado (2003), innovation in the chemical industry is influenced by many factors, including the demand and supplier-client relationships. By extending the principle of responsibility, the aim of REACH is to place the environmental impact of the activity throughout the production chain, and to change the demand of downstream users towards environmentally friendlier products. The extension of the principle of responsibility is accompanied by the obligation to communicate in the supply chain. According to the Eurostat report (2009), many companies state a positive impact on innovation of that communication. “The communication in the supply chain provides chemical companies with new information about customers and their needs”. This illustrates the importance of information in the innovation process as well as the need for coordination and collective action to spur innovation.

Since the introduction of REACH, organic solvents are subject to the authorization procedure which requires producers to develop and adopt alternatives. **Bio-solvents** are good candidates to replace organic solvents since they are less toxic, have lower VOCs emissions and are biodegradable (IRSST, 2010). Because of the extended producer responsibility, downstream users are now induced to change their preferences and to transmit their needs to suppliers regarding product quality constraints that must be achieved with alternative solvents. REACH can thus involve innovation in the product chain favored by a partnership and a support from users in the experimentation stage of the new processes for the concerned applications. We argue that our ABM model can enable to illustrate how REACH can stimulate the development and adoption of **alternatives to organic solvents**.

3 THE MODEL

In this section, we present the model we have used to analyse the impact of REACH upon innovation.

3.1 ABMs and the ODD Protocol

REACH aims at “ensuring a high level of protection of human health and the environment while enhancing innovation and competitiveness”. In order to investigate such a relationship, we use an agent-based model (ABM) because simulation models provide a powerful tool for exploring such complex systems as innovation and industrial dynamics. ABM is used to deal with complex systems made up of autonomous entities. It allows modeling the behavior of heterogeneous agents, technological diversity and the change in selection environment that result from policy measures.

The objective is to study how system level properties emerge from the adaptive behavior of individuals as well as how, in turn, the system affects individuals. This model is used as a learning tool, and is not intended for accurate prediction. It aims to provide insights about the directional effect of instruments underlying the authorization procedure of REACH on firms' innovation strategy and the associated shift to alternative substances.

In order to present the model we have built, we use the ODD protocol (Grimm et al., 2006, 2010). The ODD protocol provides a standard protocol for describing ABMs in order to make them easier to analyze, understand and communicate. The protocol consists in structuring the information about an ABM in the same sequence: Overview, Design concepts and Details (cf. Table 1). The logic behind the ODD sequence is to first provide context and general information, followed by more strategic considerations, and finally more technical details. Such a sequence allows the reader to easily absorb information in a progressive way.

Table 1: The three blocks of the ODD protocol.

Overview	Purpose
	State variables and scales
	Process overview and scheduling
Design concepts	Design concepts
Details	Initialization
	Input
	Submodels

3.2 Description of the Model

We follow the sequence given in Table 1.

3.2.1 Purpose

The purpose of our model is to understand how different configurations in the policy design of REACH affect the dynamics of eco-innovation and shape market selection and innovation.

In our model we take into account the supplier-user interactions since they represent an essential element in the development of new technologies, particularly in the chemical industry. Technological progress is driven by an endogenous stochastic innovation process relying on firms' R&D strategies. We illustrate the competition between organic solvents and biosolvents in the surface treatment activity. The objective is to examine in which extent different combinations of flexible and stringent instruments of the REACH regulation can lead to develop and diffuse alternative solvents (biosolvents).

3.2.2 State Variables and Scales

The model comprises eight low-level entities: supplier, client, two types of product (Technology 1 and Technology 2), and four product characteristics (technological performance, production cost, VOCs emissions and biodegradability).

Suppliers produce and sell products (technology 1 and/or technology 2). They are mainly characterized by the state variables: identity number and identity of the technology portfolio. Suppliers which do not perform well and do not have enough budget will exit the market; they are automatically replaced by new entrants. These new entrants are characterized by the same state variables as the suppliers. Clients buy and use one type of product (technology 1 or technology 2) in their production processes. They are characterized by the state variables: identity number, identity of the product they have bought, preferences, requirement thresholds, reservation price and minimum product quality.

There are two types of product-related technology that may co-exist: T1 (e.g. organic solvents) and T2 (e.g. biosolvents). Technology 1 is characterized by an identity number and technology 2 is characterized by an identity number and initial switching costs. At the start of the simulation run, only T1 exists and is developed by the suppliers. Each product is described by four attributes in a Lancaster way (1971): technical performance, production cost, VOCs emissions, biodegradability. Technical performance X_k is related to the solvent power and is measured by the Kauri butanol index (Kb). A good solvent power is characterized by an index of Kb greater than 100. Production costs $Cost_k$ depend on the raw materials that are used (petrol vs biomass) but also on the production facility (traditional refinery vs biorefinery). Emissions of volatile organic compounds (VOCs), $VOC_{k,}$ represent those gases and vapors containing chemical elements emitted by the solvent. VOCs are emitted during the manufacture, storage or use of the solvent. The volatility of these chemicals can have serious consequences on health and the environment. VOCs emissions are measured by the evaporation rate in kilo Pascal. Biodegradability, $Bio_{k,}$ represents the capacity of air emissions from solvents to degrade readily and to have a short atmospheric lifetime.

Each of these attributes is characterized by a potential of evolution which can be exploited by suppliers according to their R&D and innovation activities. The potential of evolution takes into account the difference in order of magnitude between the best (biosolvent) and the worst solvent (conventional solvent). Technical performance is characterized by a maximum limit X_{max}; production cost is characterized by a minimum limit $Cost_{min}$; VOCs emissions are characterized by a minimum limit VOC_{min} and biodegradability is characterized by a minimum limit Bio_{max}. These outer limits are assumed to be different depending on the technology T1 or T2. In particular, the potential of improvement regarding environmental characteristics is higher for the green technology T2 than for the conventional technology T1: $Cov_{min\ T2} < Cov_{min\ T1}$ and $Bio_{min\ T2} < Bio_{min\ T1}$. We also take into account the technology difference between T1 and T2 in the initial values. Since the green technology T2 is emergent compared to the well-established T1, we assume that T2 has a disadvantage in terms of techno-economic characteristics such that production costs are higher and technical performance is lower than T1.

3.2.3 Process Overview and Scheduling

In the model, one time step represents one period of purchase and simulations are run for 200 periods. Within each time step, six modules are processed in the following order: purchase, budget, entry/exit, technology portfolio, R&D watch/innovation, rebuy.

Purchase depends on the utility that a product, given its four attributes, brings to a client provided economic and technical constraints are first satisfied (reserve price and minimum technical quality). Once a product is selected by a client, the corresponding supplier registers a sale.

Budget of each supplier takes into account the R&D expenses and the profit derived from the sales.

Within the ***exit/entry*** module, each supplier with a negative budget exits and is replaced by a new firm so that a constant number of suppliers is observed over the whole time period. Each new entrant will be able to copy an installed firm with more or less success (absorptive capacity).

Technology portfolio enables a supplier to adopt T2 or not on the one hand and to keep or abandon T1 on the other hand so that in the end the supplier's portfolio can be constituted by T1 and/or T2.

R&D watch and innovation allow suppliers to improve the characteristics of their product. R&D watch concerns only suppliers that have not yet adopted T2 but are required (by regulation) to prove they are searching for substitutes and thus accumulate knowledge on T2. Innovation activities may then involve improvements on T1 and/or T2 depending on the technology portfolio of each supplier.

Rebuy allows each client to compare the performance achieved by its current supplier with its requirement levels. If the current supplier does not under-performs, the client keeps the same supplier;

otherwise, the client switches to a new supplier and selects one with the purchase module.

3.2.4 Design Concepts

Our model draws on basic principles developed by the evolutionary theory of technological change (Chiaromonte and Dosi, 1993); (Malerba et al., 1999, among others). Thus, a strong emphasis is put on dynamics, changing structures and disequilibrium processes with an evolutionary perspective. We find several design concepts common to ABMs in our model.

According to the evolutionary approach, *bounded rationality* characterizes economic agents that have limited cognitive capacities to collect and treat information. Suppliers seek for increased market share thanks to innovation while users seek for selecting the best product according to their preference and requirement criteria. Individuals cannot predict the future conditions they will experience; they are myopic and their decisions follow some *routines* and a satisficing principle rather than a maximizing one. In our model, suppliers make their decisions regarding technology portfolio by considering specific thresholds that reflect bounded rationality. Likewise, in the rebuy module, clients compare the performance achieved by their current supplier with their own requirement threshold and decide to keep or leave the supplier.

The decision rules are *adaptive* which means the agents adapt according to their performance and their past experience. In our model, suppliers adapt their R & D investment based on sales achieved in the past, and customers adapt their requirement levels according to suppliers' performance. *Adaptation* is thus modeled through the change in threshold levels used in the decisions of agents.

Given that decision rules are agent-specific, *heterogeneity* among individuals is a core aspect of such an evolutionary theory. Interactions between heterogeneous agents generate permanent diversity. Industry dynamics emerge from the behavior of the heterogeneous individuals.

Innovation is an endogenous and uncertain process. Indeed, firms cannot know with certainty the results of their R&D activity. That is why we model a stochastic process of innovation. Other stochastic processes are included where behavioral parameters are randomly drawn. Like the innovation process, the accumulation of knowledge that results from technology watch on T2 is stochastic. Lastly, the selection of a supplier by a client is also based on a purchase probability (reflecting errors or imperfect information).

Regarding innovation, a distinction is implicitly made between incremental and radical innovation. *Incremental* innovation allows small changes whereas *radical* innovation leads to a technological jump with significant cost and experience effects. In our model, the adoption of T2 brings radical changes that are materialized by high switching costs.

3.2.5 Initialization

At the start of a simulation run, the number of suppliers is 10 and the number of users is 200. Some initial values of the state variables are chosen randomly in a range of parameters. Others are scale parameters which have been set to plausibly calibrate the model.

For product characteristics (VOCs emissions, biodegradability, costs and technological performance), initial values are based on data to account for the difference in order of magnitude between organic solvent and biosolvent (IRSST, 2010).

3.2.6 Input Data

The model does not use input data to represent time-varying processes.

3.2.7 Submodels

Here, we specify the equations and the assumptions underlying them to better understand the modules listed in process overview and scheduling (cf. subsection 3.2.3).

Purchase: The demand for products is expressed as a demand for specific product characteristics in the Lancaster vein. The purchase probability is proportional to the utility derived by each client (*j=1,…,200*) from each product present on the market (*k=1,2*). We consider the following utility function:

$$U^{j}_{k,i,t} = \left(X_{k,i,t} - A\right)^{a} \times \left(B - P_{k,i,t}\right)^{b} \times \left(C - Cov_{k,i,t}\right)^{c} \times \left(D - Bio_{k,i,t}\right)^{d} \times \left(Ms_{i,t} + u(0,0.1)\right)^{e} \quad (1)$$

With $a, b, c, d, e \in [0,1]$. So the purchase decision depends on the performance achieved by each supplier (*i=1,…,10*) on each characteristic and on the client's preferences with respect to the product characteristics represented in the parameters *a, b, c* and *d.* A, B, C and D are technical parameters only used to avoid negative terms in the utility calculation. u(0,0.1) is drawn from a uniform distribution with values between 0 and 0.1. The parameter e can be interpreted as a bandwagon effect (Leibenstein, 1950) reflecting imitation behaviors. Indeed, there is information asymmetry regarding suppliers' performance. So clients refer to the behavior of other customers buying similar goods (Cowan et al, 1997). The clients use also the market share of the firm (Ms) which reflects the relative reputation of the supplier. The market share as an indicator provides information on the quality of the product observed by customers who have already adopted.

Each client is also supposed to be limited by economic and technical constraints. So we assume a reserve price and a minimum technical performance for each client. If one of these constraints is not satisfied when selecting a product on the market, the associated utility will be equal to zero.

The price P is deduced from the production cost by applying a mark-up rate:

$$P_{k,i,t} = (1 + \mu) \times Cost_{k,i,t} \qquad (2)$$

Where μ is a mark-up rate over production costs. For simplicity, μ is supposed to be constant and identical for every firm.

Budget: The budget B is determined by the residual budget from the previous period, the profit and the R&D expenses:
For typical suppliers:

$$B_{i,t} = B_{i,t-1} + \pi_{i,t-1} - RD_{i,t-1} \qquad (3)$$

For new T2 adopters:

$$B_{i,t} = B_{i,t-1} + \pi_{i,t-1} - RD_{i,t-1} - SC_{i,t-1} \qquad (3')$$

Where SC are the switching costs resulting from the adoption of the radically new technology T2.

The profit is determined as follows:

$$\pi_{i,t} = (\mu \times Cost_{i,t} \times Q_{i,t}) - FC \qquad (4)$$

Where $Q_{i,t}$ is the total number of products sold by firm *i;* FC are the fixed costs which are supposed to be identical for all the firms for simplicity reasons.

***Entry/Exit Processes*:** Firms with a negative budget B go bankrupt and disappear from the market. When one firm exits the market, we assume that a new firm enters so that the number of firms in the industry is kept constant.

Entry occurs with a new firm imitating an existing one. This choice is based on probabilities proportional to the installed firms' market shares. The new firm copies the technology portfolio and the product characteristics of the imitated firm. We assume that the new firm has an absorptive capacity which enables her to copy the attributes of the imitated firm in a range of [0.8;1.2]. This allows the new entrant to under-perform or inversely to over-perform in comparison with the imitated firm.

The initial budget (B) and the initial fixed costs (FC) of the new firm are set in the same way as for the firms created at the start of a simulation run. The knowledge stock (K) and the switching costs (SC) of the new firm are function of the industry average.

***Technology Portfolio*:** Every period, firms examine the possibility to change their technology portfolio. They compare an adoption index with a certain threshold.

When T2 has not yet been adopted by anyone, we have the following adoption index:

$$AdIndex_{i,t}^{T2} = K_{i,t-1} \times (\varphi) \qquad (5)$$

K stands for the knowledge stock cumulated on the green technology T2 derived from the firm's activity of technological watch. φ is a parameter reflecting the "first-mover advantage" i.e. the advantage gained by the very first firm adopting T2.

When T2 has already been adopted, the probability that a firm adopts the green technology T2 depends on the following adoption index:

$$AdIndex_{i,t}^{T2} = K_{i,t-1} \times (Ms_{t-1}^{T2}) \qquad (5')$$

Ms^{T2} represents the total market share of the Green technology T2. Thus the probability to adopt T2 depends positively on the stock of knowledge K accumulated on T2 but also on how T2 has diffused on the market.

The decision to adopt T2 follows a two steps procedure. First, the firm compares its adoption index with an adoption threshold under which the firm will not adopt T2. If its adoption index is above the threshold, then the second step determines if the firm has a sufficient budget to bear the switching costs related to the green technology.

For firms that decide to adopt the green technology, they can continue to produce and sell the conventional technology T1. They will have a technology portfolio constituted of T1 and T2. However firms can decide to abandon the conventional technology and focus only on the development of the green technology T2. Here we assume that firms calculate the return on investments of technology T1 and compare it with a certain threshold. The return on investment is based on the ratio:

$$ROI_{i,t}^{T1} = \frac{P_{i,t-1}^{T1} \times Q_{i,t}^{T1}}{RD_{i,t-1}^{T1}} \qquad (6)$$

The ratio turnover/R&D gives an indication of the ability of the technology to recover one euro spent in R&D in the total return. The lower the return on investment of technology T1 compared to the minimum threshold, the higher the likelihood to be abandoned.

Innovation Process and Green Technological Watch: At each period, every firm can improve the product performance in their portfolio by carrying out R&D and innovation activities.

Every firm will allocate a certain proportion δ of its budget to R&D activities:

$$RD_{i,t} = \delta \times B_{i,t} \tag{7}$$

Then, each firm is assumed to split its global R&D budget between both technologies T1 and T2:

$$RD1_{i,t} = \delta_1 \times RD_{i,t} \tag{8}$$

$$RD2_{i,t} = (1 - \delta_1) \times RD_{i,t} \tag{9}$$

Where δ_1 is the share of total R&D allocated to R&D1 (technology T1).

For firms developing only the green technology T2, $\delta_1 = 0$. For firms developing both technologies T1 and T2, $\delta_1 = 0.5$. For firms developing only the conventional technology T1, $\delta_1 = 0.5$ since they devote the other part to technological watch on the green technology T2 (RDwatch).

R&D watch follows a stochastic process. Success occurs if the following condition is satisfied:

$$1 - e^{-\alpha_w \times RDwatch_{i,t}} \geq u(0,1) \tag{10}$$

Where α_w is a scale parameter determining the speed at which the level of the current R&D expenditure allows knowledge accumulation and $RD2_{i,t}$ represents R&D expenses allocated to technology 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 (10) with a given R&D investment.

In case of success, new knowledge on T2 is accumulated and the switching costs linked to the potential adoption of T2 decrease.

$$K_{i,t} = K_{i,t-1} + \alpha_K \times u(0,1) \times \left(Kmax - K_{i,t-1}\right) \tag{11}$$

$$SC_{i,t} = SC_{i,t-1} - \alpha_{sc} \times u(0,1) \times (SC_{t-1} - SCmin) \tag{12}$$

Where α_K and α_{sc} are scale parameters.

The innovation process is similar to the previous procedure. Two steps are considered for each product characteristic. First, the innovation probability depends on the R&D investment allocated to the technology. Success of innovation depends on the following condition:

$$1 - e^{-\alpha_I \times RD_{k,i,t}} \geq u(0,1) \tag{13}$$

Where α_I represents the speed of the innovation process and $RD_{k,i,t}$ the R&D expenses devoted by firm *i* to product *k* at time *t*.

Then, in case of success, the outcome of innovation needs to be calculated. For the different characteristics, we have:

$$\Delta X_{k,i,t} = \beta_1 \times u(0,1) \times \left(Xmax - X_{k,i,t-1}\right) \tag{14}$$

$$\Delta Cost_{k,i,t} = \beta_2 \times u(0,1) \times \left(Cost_{k,i,t-1} - Costmin\right) \tag{15}$$

$$\Delta VOC_{k,i,t} = \beta_3 \times u(0,1) \times \left(Cov_{k,i,t-1} - Covmin\right) \tag{16}$$

$$\Delta Bio_{k,i,t} = \beta_4 \times u(0,1) \times \left(Bio_{k,i,t-1} - Biomin\right) \tag{17}$$

Where $\beta_{1,}$ β_2, β_3 *and* β_4 are scale parameters; u(0,1) is a uniform random value selected between 0 and 1 which reflects the efficiency of the R&D activity and thus impacts the innovative outcome. The last term of the equation represents the distance to the technological frontier associated to each product characteristic. By doing so, when the level of a given product characteristic comes closer and closer to the limit of what is achievable with the considered product design, a given R&D expenditure will achieve less and less further progress (lower technological opportunities and R&D decreasing returns).

Rebuy: each client *j* is assumed to use one single product at the same time and to renew its purchase every period. When renewing the product, the client compares its minimum thresholds on each characteristic with the performance actually achieved by its current supplier. Requirement thresholds change with the average performance in the industry. For the technical performance criteria,

$$\begin{aligned} Lim\_minX^j_{k,i,t} = Lim\_minX^j_{k,i,t-1} + \varepsilon \\ \times \left[max\left(0, a \times (\bar{X}_{k,t} - Lim\_minX^j_{k,i,t-1})\right)\right] \end{aligned} \tag{18}$$

And so on for the other criteria (equations 19, 20 and 21). The parameters *a, b, c* and *d* represents the client's preferences for the considered characteristic; ε is a scale parameter; for each product *k*, the average performance of industry on each characteristic is given by:

$$\bar{X}_{k,t} = \textstyle\sum_{i=1}^{N} X_{k,i,t}/N;\ \overline{VOC}_{k,t} = \sum_{i=1}^{N} VOC_{k,i,t}/N;$$
$$\bar{P}_{k,t} = \textstyle\sum_{i=1}^{N} P_{k,i,t}/N;\ \overline{Bio}_{k,t} = \sum_{i=1}^{N} Bio_{k,i,t}/N$$

If one of the minimum thresholds is not met (i.e. is below the current supplier's performance), then the client leaves the current supplier and chooses another one through the purchase procedure.

4 RESULTS

Before presenting the results of our simulations, we first expose the simulation protocol we have followed

4.1 The Experimental Protocol

Results are analyzed through specific indicators and are based on a high number of simulations in order to deal with stochastic processes.

4.1.1 Main Indicators Characterizing the Industrial Dynamics

The following indicators are used to exhibit the main characteristics of the industrial dynamics:

- The inverse Herfindahl-Hirshman index of concentration (1/HHI with HHI the sum of the squares of the firms' market shares), which value is comprised between 1 (monopoly) and N (atomicity). The higher invHHI the higher the degree of competition and inversely;
- The number of failures, which takes into account the number of exiting firms in each period. In our model, the higher the number of failures, the higher the number of new entrants that come and replace the exiting firms;
- The respective market share of technology T1 and technology T2;
- A global environmental indicator which traces back the stock of VOCs emissions at the industry level. We consider the following equation:

$$VOCStock_t = VOCStock_{t-1} - ABS + \sum_{j=1}^{M} VOC_{k,t}^{j} \times Bio_{k,t}^{j} \qquad (22)$$

Where *ABS* stands for the assimilative capacity of an ecosystem receiving pollution (VOCs emissions) at each period. It is set exogenous and constant over time. According to equation (22), the current stock of VOCs emissions depends on the previous stock of VOCS (the 'history' of pollution flows) less assimilated emissions by the ecosystem plus the current flow of emitted VOCs. Such a global environmental indicator enables to grasp the ability of the industry to decrease its VOCs emissions over time. Such a decrease in VOCs can result from two effects: a qualitative effect through innovation (decrease in the VOC and/or Bio characteristics) and a quantitative effect through lower market size in the case where clients cannot afford the product (too costly and/or too low quality).

4.1.2 The Baseline Simulations and the Regulation Module

The baseline simulations serve as a *benchmark* to study the effect of regulation upon industrial dynamics. In order to cope with stochastic processes, the results of our benchmark are drawn from a battery of 500 simulations. For each indicator, the average over 500 simulations is computed at different time steps: 0, 50, 100, 150 and 200.

The *regulation module* includes the authorization procedure and the extended responsibility principle. The purpose of the **authorization** process is to progressively replace substances of very high concern by other substances or technologies where these are economically and technically viable. Two action leverages are considered in our model.

First, **target-thresholds** for techno-economic performances of alternative solutions (X* and Cost*) are incorporated. If technology T2 reaches both thresholds of technical and economic performance, then the public authorities can consider the existence of viable solutions and can prohibit the use of technology T1 after **the sunset date**. On the contrary, if technology T2 does not reach the target thresholds, the public authorities can consider that there are no techno-economically viable alternatives. In that case, authorizations are granted and firms can use technology T1 after the sunset date, but *only if* they prove that they carry out serious analyses of alternatives providing information on their R & D activity.

In our model, the budget allocated to **R&D watch on T2** is used to check whether a firm is searching for new alternatives. Below a certain threshold, authorization will not be granted. Above the threshold, authorizations are granted for a period and can be **reviewed** if "new information on possible substitutes is available". The threshold for R&D watch depends on the average R&D watch performed in the industry multiplied by a parameter ($\alpha_{RDwatch}$*) which value expresses the degree of severity of regulation (the closer to 1 the stricter the regulation, the closer to 0 the softer the regulation).

The **timing of regulation** is the second action leverage for public authorities. Indeed an early sunset date associated to close revision dates can be considered to be strict. On the contrary a late sunset date and distant revision dates impose softer constraints. In order to take timing into account, we assume that the probability to adopt technology T2 (equation 5') is modified as follows:

$$AdIndex_{i,t}^{T2} = K_{i,t-1} \times (Ms_{t-1}^{T2}) \times \left[(1 + \alpha_{R}^{i}) \times \frac{t}{T}\right] \qquad (5'')$$

The meaning of T and thus its value depends on whether it is the first time a deadline is given to firms before public authorities check the existence of suitable alternatives (in such a case, T=the sunset date, T_{sunset}) or if authorization has been granted and subsequent checks will be carried out (in such a case T=the revision date, $T_{revision}$). α^i_R is a parameter reflecting the credibility that a firm *i* confers to regulation (ranges between 0 and 1).

With equation (5''), we thus assume that regulation positively influences the adoption of the green technology T2: the earlier and the closer to the sunset date, the higher the adoption index; the more frequent the revision of authorization the higher the adoption index; the higher the credibility given to regulation, the higher the adoption index.

By extending the **responsibility principle**, REACH aims at changing the demand of downstream users of chemical products towards less toxic and harmful substances. In order to take into account such a change in our model, we will now consider that the technology portfolio hold by suppliers matters in the clients' decisions such that: first, the utility of a product (equation 1) will tend to decrease for suppliers which portfolio is only constituted by technology T1; in that case the utility is weighted by a factor $\left[\left(1-\alpha^j_R\right)\times\frac{t}{T}\right]$ where α^j_R is a parameter reflecting the credibility that a client *j* gives to regulation (ranges between 0 and 1) and T will represent alternatively the sunset date or the revision date; second, the decision made by a client to leave its current supplier will be subject to a probability of defection based on $\left[\left(\alpha^j_R\right)\times\frac{t}{T}\right]$ when the supplier's portfolio is only constituted by technology T1. According to these changes, the closer the sunset date or the revision date, the lesser the weight given to suppliers holding a portfolio with only technology T1 in the calculation of utility (equation 1) in the purchase module but also in the update of requirements in the rebuy module (equations 20 and 21).

4.2 The Impact of Regulation upon the Market Dynamics

In the following, we study **two opposite configurations** (cf. Table 2), the "less stringent scenario" and the "most stringent scenario", depending on the target-thresholds and on the timing of regulation.

4.2.1 Initialization

The initial values for techno-economic performances are chosen in relation with the size of the techno-economic potential which can be covered by innovators. In the low stringency configuration, 90% of the potential must be covered while in the high stringency configuration 10% needs to be covered.

Table 2: Policy variables in the REACH model.

Scenario / Policy variables		Less stringent	Most stringent
Target-thresholds	Techno-eco performances	High X*	Low X*
		Low Cost*	High Cost*
	R&D watch	$\alpha_{R\&Dwatch}$* close to 0	$\alpha_{R\&Dwatch}$* close to 1
Timing	Sunset date	T_{sunset} late	T_{sunset} early
	Revision date	$T_{revision}$ distant	$T_{revision}$ close

The mechanism is the following: at the sunset date, if the average cost of T2 is below the corresponding target-threshold *and* the average technical performance of T2 is above the corresponding target, then T1 is forbidden for every firm in the industry. If not, the budget of R&D watch is checked for each firm. If such a budget is below a certain threshold, then T1 is forbidden for the considered firm. If not, it is possible to continue developing T1 as if the authorization had been individually granted until a certain period of time. At the revision date, a similar sequential checking is made.

4.2.2 Main Results

The graphs below depict the evolution of each indicator in the different cases: the benchmark scenario (black line), the less stringent scenario (grey dotted line) and the most stringent scenario (grey full line).

Results show that regulation increases industrial concentration all the more strongly that regulation is more stringent (cf. Figure 2).

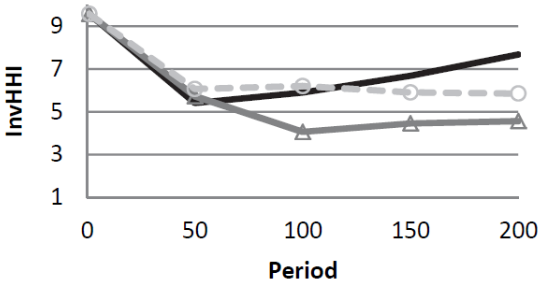

Figure 2: Evolution of the inverse HHI (average for 500 simulations).

Figure 3 shows that regulation helps technology T2 to take off and to increase its market share compared to the benchmark scenario where T2 was doomed to a niche (12% in average at t=200). However, only the most stringent scenario allows domination of T2 due to an early ban of T1 (in t=50).

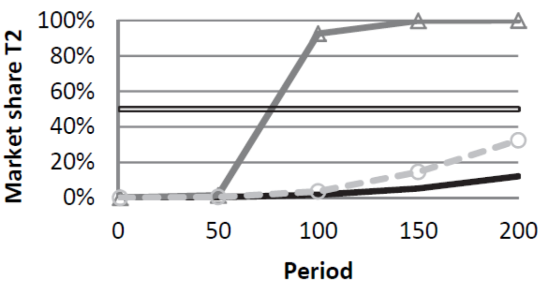

Figure 3: Evolution of market shares for T2 (average for 500 simulations).

As to the stock of VOCs, we observe a kind of inverted U curve in the most stringent scenario as VOCs emissions rise in a first place and then fall with the advances of innovation and the diffusion of T2 but also with a decrease in market size (cf. Figure 4). By contrast, the less stringent scenario exhibits systematically higher levels of VOCs over time compared to the benchmark. This is due to the fact that firms specialised on T1 (and very efficient in improving the product characteristics) are disturbed by regulatory mechanisms during the whole time period without yet experiencing complete prohibition of T1.

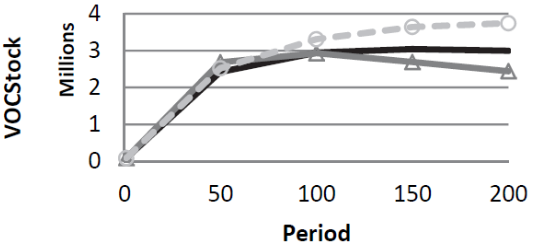

Figure 4: Evolution of the global stock of VOCs (average for 500 simulations).

In our model, failures result from a combination of different effects: low sales (and thus insufficient budget) and attachment of clients to their suppliers (fidelity effect) that both prevail in the benchmark scenario; forced exit due to not enough R&D watch on T2 or to T1 ban when regulation is incorporated. Results show that the number of failures due to this combination of effects is much higher in the most stringent scenario than in the benchmark while it is lower in the less stringent scenario (cf. Figure 5).To summarize, we see that the most stringent scenario characterized by strict timing (early sunset date and frequent revisions) and strict techno-economic performances for alternative substances (low price-quality ratio for T2) pushes radical environmental innovation by allowing strong and early take-off of technology T2 and prohibition of technology T1. But being detrimental to incremental innovation on T1, such a scenario leads to lower global environmental performances (higher stock of VOCs) in the short term. This illustrates the tension between the short and the long term underlying the development of radical environmental technologies.

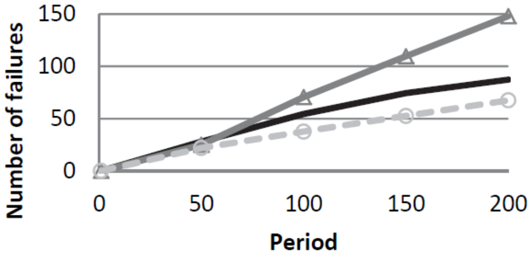

Figure 5: Evolution of failures (average for 500 simulations).

5 CONCLUSIONS

This paper intends to contribute to a better understanding of the relationship between policy design and eco-innovation through an agent-based model. Stringency, flexibility and timing of regulation are crucial to spur eco-innovation. These are key aspects to consider in the REACH regulation, especially to foster the development of alternative substances (like biosolvents) to replace toxic and harmful substances (like organic solvents).

The ABM model we propose in this paper is original in many aspects: evolutionary modeling of innovation and industrial dynamics; vertical interactions between suppliers and users; technology portfolio; authorization procedure and extended producer responsibility. The model is used as a learning tool, and is not intended for accurate prediction. It aims to provide insights about the directional effect of instruments underlying the authorization procedure of REACH on firms' innovation strategy and the associated shift to alternative substances.

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