



# L'écoconception, voie de la transition pour une chimie durable

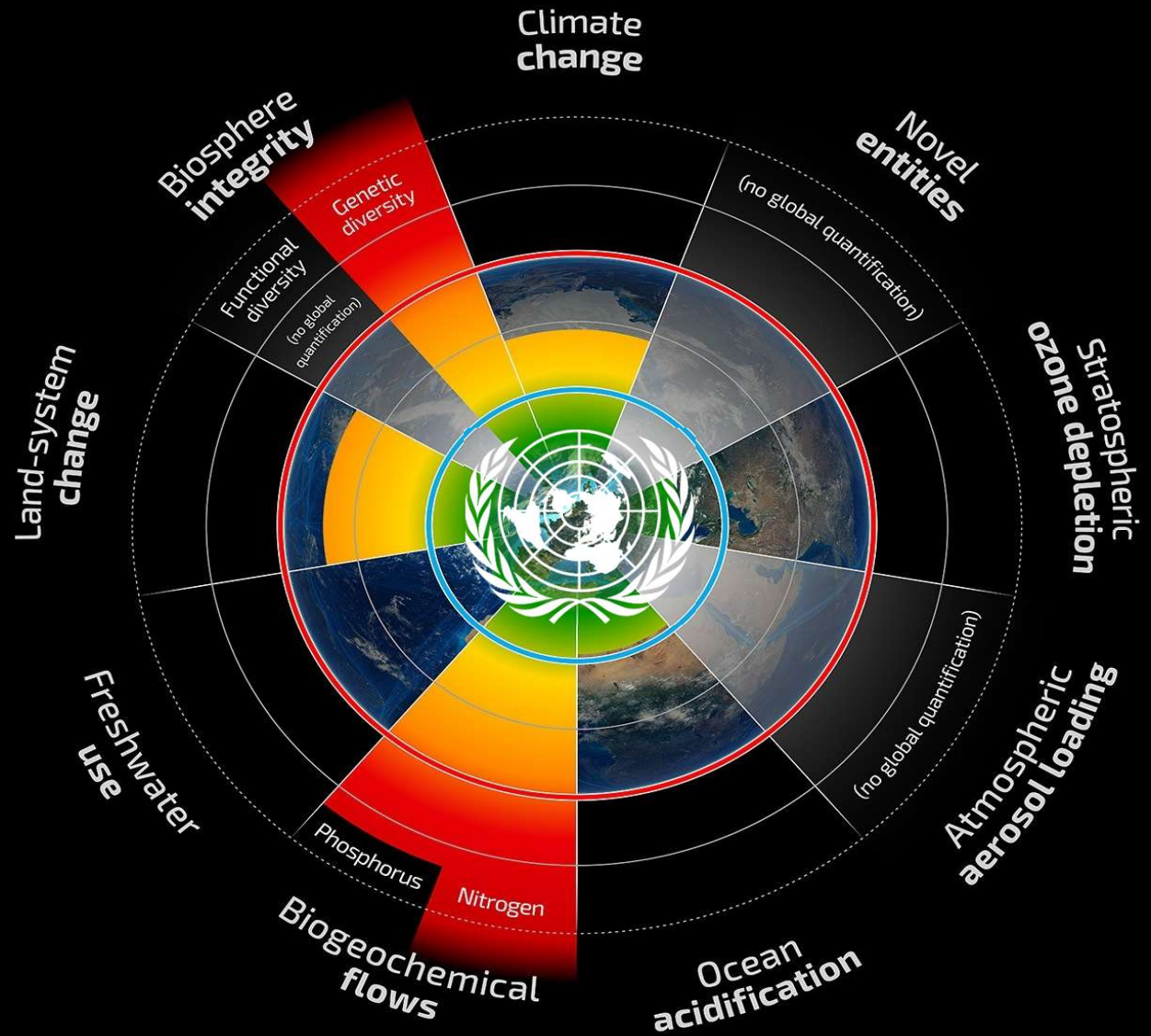
## Les mardis de la Chimie Durable

(Webinaire 16.01.2024)

M. Philippe PhD,  
*Consultant in Eco-design, Green Chemistry and Naturalness*  
Ex-L'Oréal Fellow  
[michel.philippe7@wanadoo.fr](mailto:michel.philippe7@wanadoo.fr)

-M. Philippe 16.01.2024

# PLANETARY BOUNDARIES



Rockström and al. Planetary boundaries : exploring the safe operating space for humanity.  
*Ecology and Society* 2009 14(2): 32.  
<http://www.ecologyandsociety.org/vol14/iss2/art32/>



# HOLISTIC THINKING

-M. Philippe 16.01.2024

# MAJOR STAKEHOLDERS' CONCERNS *AROUND BIODIVERSITY*

- Deforestation
- Marine & freshwater pollution
- Illegal trade / extinction of emblematic endangered species
- Natural resources depletion
- Overfishing/marine resources
- GMO & Bio-engineering
- Pesticides (bees collapse)
- Farmers rights , patents on seed (biopiracy)
- Land use conflicts



# **BIODIVERSITY LOSS** *IS ALSO A SOCIAL ISSUE*

- Humans depends on natural resources such as water, arable land, fish and wood; and **ecosystem services** such as pollination, nutrient cycling and erosion control
- Biodiversity decline is greater in the tropics
- **Low-income countries** have the smallest footprint, but suffer the **greatest ecosystem losses**

**The world's poorest continue to be most vulnerable to biodiversity loss**



**« C'EST UNE TRISTE CHOSE DE SONGER QUE LA  
NATURE PARLE ET QUE LE GENRE HUMAIN N'ECOUTE PAS »**

**VICTOR HUGO, "CARNETS", 1870**





## ***WHAT'S GREENWASHING?***

**HIDDEN TRADE OFF = Compromis caché**

**NO PROOF = Absence de preuves**

**VAGUENESS = Imprécision**

**IRRELEVANCE = Non-pertinence**

**LESSER OF 2 EVILS = Moindre de 2 maux**

**WORSHIPING FALSE LABELS = Culte de l'étiquette mensongère**

**FIBBING = Mensonge**





# Principles of the UN Global Compact

(derived from the Rio Declaration on Environment and Development)

## On the Environment

- ▶ **Principle 7:** Businesses should support a precautionary approach to environmental challenges;
- ▶ **Principle 8:** undertake initiatives to promote greater environmental responsibility;
- ▶ **Principle 9:** encourage the development and diffusion of environmentally friendly technologies.

## SUSTAINABLE DEVELOPMENT GOALS



# The Science Based Targets initiative (SBTi) drives ambitious climate action in the private sector by enabling organizations to set science-based emissions reduction targets

The SBTi's target dashboard shows science-based targets set and commitments made by companies and financial institutions since 2015.

It provides details of all organizations that are working to reduce their emissions by setting science-based targets. This includes the 'target wording': Details of the specific emissions reductions organizations must make that have been independently assessed and validated as science-based by the SBTi.

- **Targets** are clearly-defined pathways for companies and financial institutions to reduce greenhouse gas (GHG) emissions, which have been validated by the SBTi. Details of an organization's target can be viewed by expanding the rows below.

- **Commitments** demonstrate organizations' intention to develop targets and submit these for validation within 24 months. They are indicated by the word 'committed' in the dashboard. Making a commitment is the first step in setting a science-based target; organizations with the word 'committed' have not yet set a target.

<https://sciencebasedtargets.org/>

# The European Green Deal



# DE L'ÉCOCONCEPTION DES PRODUITS AU PACTE VERT EUROPÉEN

**L'écoconception** à travers le biomimétisme avec l'aide essentielle de la chimie verte bio-inspirée, de la biotechnologie et le développement des voies circulaires de synthèse est :

**Une approche innovante et nécessaire pour développer la **Chimie Durable** en respect du Pacte Vert Européen :**

[https://commission.europa.eu/strategy-and-policy/priorities-2019-2024/european-green-deal\\_fr](https://commission.europa.eu/strategy-and-policy/priorities-2019-2024/european-green-deal_fr)

- Initiation en 2019
- Neutralité climatique visée en 2050



Supplying clean, affordable and secure energy

A zero pollution ambition for a toxic-free environment

Preserving and restoring ecosystems and biodiversity

## Importance de l'Ecoconception

La définition officielle pour l'ADEME est la suivante :

- ▶ « C'est une démarche **préventive** et innovante qui permet de réduire les impacts négatifs du produit, service ou bâtiment sur l'environnement sur l'ensemble de son cycle de vie, tout en conservant ses qualités d'usage »
- ▶ L'écoconception est une approche qui prend en compte les impacts environnementaux dans la **conception** et le **développement** du produit et ceci tout au long de son cycle de vie: **de la source de la matière première**, à la **fin de vie** en passant par la fabrication, le transport et l'usage

For ISO 14006:2020 standard:

- ▶ Eco-design is based on a **preventive** and **innovative** approach which considers environmental aspects in design and development with the aim **to reduce adverse environmental impacts** throughout the life cycle of a product.



## DE L'ÉCOCONCEPTION DES PRODUITS AU PACTE VERT EUROPÉEN

- ❑ **Travailler avec la nature pour protéger notre planète et notre santé**



- ❑ **Renforcer l'action mondiale pour le climat**



# FEUILLE DE ROUTE POUR L'INDUSTRIE CHIMIQUE DE L'U.E.

*La Commission et les parties prenantes ont utilisé les thèmes clés de huit éléments de base pour élaborer une feuille de route pour l'industrie chimique de l'UE. Le résultat est une feuille de route composée de trois composantes, comme indiqué ci-dessous:*

- ▶ •1. Une composante axée sur l'action regroupant les sujets sous trois thèmes transversaux : **la collaboration pour l'innovation, l'approvisionnement en énergie propre et la diversification des matières premières**. Le choix de ces thèmes a été éclairé par l'analyse de la documentation existante et la discussion avec les différents intervenants.
- ▶ •2. **Une composante technologique** qui donne un aperçu des différents sujets liés à la technologie comme contribution à la transition.
- ▶ 3. Une composante réglementaire qui recueille la législation existante - y **compris les grandes initiatives de R&I influençant les développements dans l'industrie chimique**.

✓ *En mettant en œuvre les actions identifiées sous chaque thème, l'industrie chimique accélérera la double transition et améliorera sa résilience, sa durabilité et sa circularité conformément au Pacte vert européen.*







# Green and Digital Transition



*Figure 2 - The 8 building blocks considered to develop the transition pathway for the chemical industry*



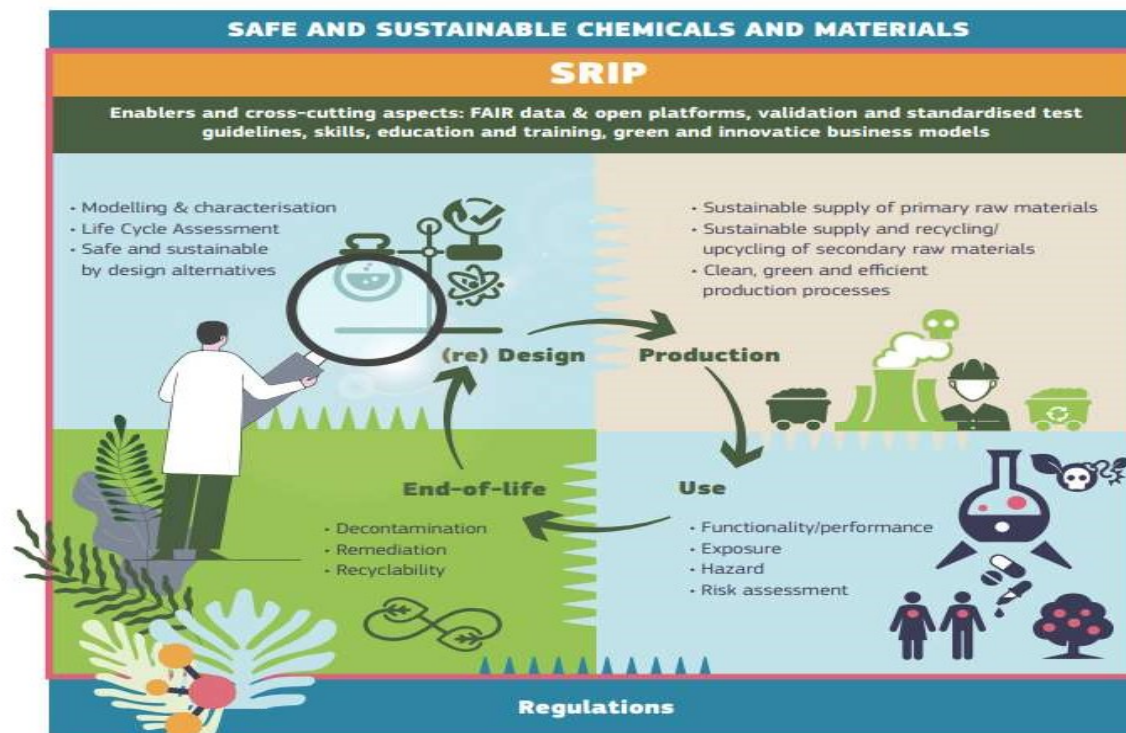
## 2) TECHNOLOGY ROADMAP

<b>EU Initiatives supporting Technological Transition</b> <i>(SET Action Plan)</i>	<b>Actions</b> <i>(as presented in Building Blocks – Part II)</i>	<b>EU Initiatives</b>
 <b>A) ELECTRIFICATION</b>	6.2. Develop hub structures 8.3. Development of an industrial technology roadmap 14. Anticipate I-t needs for the supply of energy and feedstock resource 15.1. Channel investments for clean energy 15.2. Ensure competitive supply of clean energy 15.3. Improve Power-Purchase Agreements 18.1 Enable the free flow of energy between countries 20.1. Increase availability and capacity of multi-modal terminals close to industrial clusters 20.2. Improve use of rail transport	<ul style="list-style-type: none"> <li>• REPowerEU</li> <li>• EU Renewable Directive</li> <li>• TEN-E Regulation</li> <li>• Proposal for a directive on Energy Efficiency</li> </ul>
 <b>B) HYDROGEN</b>	6.2. Develop hub structures 6.3. Manage and convert existing assets 15.1. Channel investments for clean energy 15.2. Ensure the competitive supply of clean energy 18.2. Develop a separate hydrogen infrastructure at EU level	<ul style="list-style-type: none"> <li>• European Clean Hydrogen Alliance</li> <li>• Hydrogen and decarbonised gas market package</li> </ul>
 <b>C) BIOMASS</b>	4.3. Strengthen initiatives with SMEs under the EIC 8.1. Promote safety and sustainability assessment approaches 9.1. Foster collaboration and partnerships 16.2. Biomass as an alternative feedstock 19.1. Develop recycling facilities and bio-refineries (and exploit synergies with the chemical industry)	<ul style="list-style-type: none"> <li>• Revision of the Renewable Energy Directive</li> <li>• INCITE (Industrial Emissions Directive)</li> </ul>
 <b>D) WASTE</b>	3.2 Improve collaboration in value chains 3.3 Support product design and re-design 8.1. Promote safety and sustainability assessment approaches 11.1. Definitions and concepts 11.2. Methods 16.3. Waste as an alternative feedstock 22.1. Set a regulatory framework for the transport of waste 22.2. Improve the management of logistics for waste feedstock	<ul style="list-style-type: none"> <li>• Hubs4Circularity</li> <li>• Waste Framework Directive</li> <li>• Landfill Directive</li> </ul>
 <b>E) CCU &amp; CCS</b>	6.3. Manage and convert existing assets 9.2. Support for development 16.4. CO <sub>2</sub> as an alternative feedstock 22.2. Improve the management of logistics for waste feedstock	<ul style="list-style-type: none"> <li>• Hubs4Circularity</li> <li>• Sustainable Carbon Cycle</li> </ul>
 <b>F) PROCESS EFFICIENCY</b>	3.2 Improve collaboration in value chains 3.3 Support product design and re-design 5.1. Facilitate exchange of information (new synergies) 5.3. Support the development of Partnerships for Innovation 6.3. Manage and convert existing assets 17. Process efficiency 19.1. Develop recycling facilities and bio-refineries (and exploit synergies with the chemical industry) 20.1. Increase the availability and capacity of multi-modal terminals that are close to industrial clusters 21.2. Deploy technologies to improve chemical manufacturing processes and data gathering 25.2. Safety and social security of workers	<ul style="list-style-type: none"> <li>• REPowerEU</li> <li>• Industrial Symbiosis</li> <li>• Revision of the Industrial Emission Directive</li> </ul>

# QUEL PLAN STRATEGIQUE POUR DEVELOPPER LA RECHERCHE ET L'INNOVATION?

# PLAN STRATEGIQUE EUROPEEN pour La RECHERCHE ET L'INNOVATION (SRIP)

**Figure 1:** The life-cycle approach of the Strategic Research and Innovation Plan (SRIP)



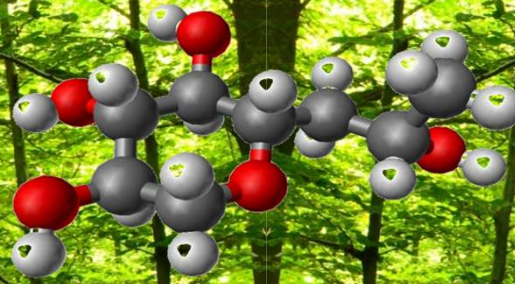
**Figure 1:** The life-cycle approach of the Strategic Research and Innovation Plan (SRIP). The Plan focuses on enabling and crosscutting aspects and R&I needs in line with life cycle stages of chemicals and materials. As chemicals and materials are used in many different sectors and consumer goods the identified R&I areas can also contribute to increasing the overall sustainability of these value chains and products.

# L'ECOCONCEPTION pour un Faible Impact et un Caractère DURABLE

- ▶ •Modélisation, Méthodes Prédicatives et Caractérisation (molécules ciblées, procédés...)
- ▶ •Évaluation du cycle de vie global (ex.: filières, sourcing durable, recyclage...)
- ▶ •Développement d'alternatives sûres et durables par l'écoconception (matières premières, procédés...)

# Processus et technologies de production sûrs et durables

- ▶ • Approvisionnement durable en matières premières primaires
- ▶ • Recyclage des matières premières secondaires, co-produits
- ▶ • Des processus de production propres, écologiques et efficaces à faible impact



## Importance of Ecodesign through Green Chemistry/Biotechnology with the help of Metrics

*"If you can not measure it, you can not improve it."* (Lord Kelvin)



# COMMITMENT TO *GREEN & SUSTAINABLE CHEMISTRY AND BIOTECHNOLOGY*

- To ensure maximum human and environmental health and safety  
    « **Safe by Design** »
- To develop innovation

Following the basic  
**GREEN CHEMISTRY** principles,  
published by P. T. Anastas and J.C. Warner

## 12 Principles of Green Chemistry

(Anastas P., Warner J.C., Green Chemistry, Oxford University Press, New-York, 1998, p.30)

- 1. Prevention** - It is better to prevent waste than to treat or clean up waste after it has been created.
- 2. Atom Economy** - Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.
- 3. Less Hazardous Chemical Synthesis** - Wherever practicable, synthetic methods should be designed to use and generate substances that possess little or no toxicity to human health and the environment.
- 4. Designing Safer Chemicals** - Chemical products should be designed to effect their desired function while minimizing their toxicity.
- 5. Safer Solvents and Auxiliaries** - The use of auxiliary substances (e.g., solvents, separation agents, etc.) should be made unnecessary wherever possible and innocuous when used.
- 6. Design for Energy Efficiency** - Energy requirements of chemical processes should be recognized for their environmental and economic impacts and should be minimized. If possible, synthetic methods should be conducted at ambient temperature and pressure.
- 7. Use of Renewable Feedstocks** - A raw material or feedstock should be renewable rather than depleting whenever technically and economically practicable.
- 8. Reduce Derivatives** - Unnecessary derivatization (use of blocking groups, protection/ deprotection, temporary modification of physical/chemical processes) should be minimized or avoided if possible, because such steps require additional reagents and can generate waste.
- 9. Catalysis** - Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.
- 10. Design for Degradation** - Chemical products should be designed so that at the end of their function they break down into innocuous degradation products and do not persist in the environment.
- 11. Real-Time analysis for Pollution Prevention** - Analytical methodologies need to be further developed to allow for real-time, in-process monitoring and control prior to the formation of hazardous substances.
- 12. Inherently Safer Chemistry for Accident Prevention** - Substances and the form of a substance used in a chemical process should be chosen to minimize the potential for chemical accidents, including releases, explosions, and fires.

# EVALUATION DU RISQUE: METHODOLOGIE

- ▶ Regroupement des produits chimiques : élaborer des approches efficaces et mécanistes, y compris l'utilisation de l'intelligence artificielle, pour regrouper les produits chimiques, appuyées par des données suffisantes sur le devenir, le potentiel de bioaccumulation et les prédictions (éco)toxicologiques
- ▶ Amélioration des méthodologies et des outils : traitement des performances, faisabilité réglementaire, conformité légale, protection, exigences en matière de données et fiabilité des conclusions
- ▶ Approches ciblées : traiter les contaminants de préoccupation émergente, les substances persistantes, mobiles et toxiques (PTM) et les perturbateurs endocriniens afin d'améliorer la couverture des compartiments environnementaux vulnérables
- ▶ Partage de l'information : élaborer des outils et des lignes directrices pour le partage de l'information et des données
- ▶ Renforcement de la confiance et communication des risques : inclure la recherche en sciences sociales et humaines pour aider à accroître la transparence, la fiabilité et la confiance (y compris les facteurs de confiance) dans les évaluations des risques et son rôle dans la protection de la société



# Évaluation des risques environnementaux et toxicologiques

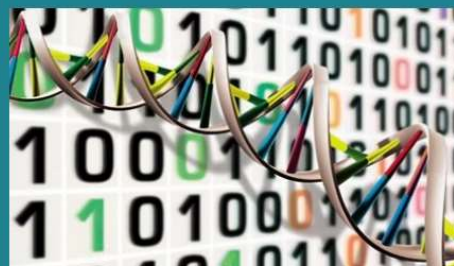
- ▶ Évaluation intégrée des dangers
- ▶ Données toxicocinétiques
- ▶ Modèles et tests (éco)toxicité
- ▶ Evaluation robuste de la toxicité des matières de taille micro/nanométrique ( ex., microplastiques, nanomatériaux)
- ▶ Mélanges : étude des propriétés (éco)toxicologiques des mélanges (involontaires et intentionnelles) et des constituants qu'ils contiennent
- ▶ Bases de données : construire une base de données ouverte des interactions synergiques et antagonistes des substances
- ▶ Analyse des données : utiliser l'intelligence artificielle pour établir des mécanismes de risque, y compris pour les mélanges



<https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test>

## User's Guide for T. E. S. T. (Toxicity Estimation Software Tool) Version 5.1

*A Java Application to Estimate Toxicities and  
Physical Properties from Molecular Structure*



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## US EPA Toxicity Estimation Software Tool (TEST) (2)

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- Hierarchical clustering method: The toxicity for a given query compound is estimated using the weighted average of the predictions from several different models. The different models are obtained by dividing the training set into a series of structurally similar clusters.
- Single model method: Predictions are made using a multilinear regression model that is fit to the training set (using molecular descriptors as independent variables)
- Group contribution method: Predictions are made using a multilinear regression model that is fit to the training set (using molecular fragment counts as independent variables).
- Nearest neighbor method: The predicted toxicity is estimated by taking an average of the 3 chemicals in the training set that are most similar to the test chemical.
- Consensus method: The predicted toxicity is estimated by taking an average of the predicted toxicities from the above QSAR methods.



# OECD QSAR TOOLBOX

# OECD Principles for the Validation, for Regulatory Purposes, of (Q)SAR Models

- ▶ a defined endpoint
- ▶ an unambiguous algorithm
- ▶ a defined domain of applicability
- ▶ appropriate measures of robustness and predictivity
- ▶ a mechanistic interpretation

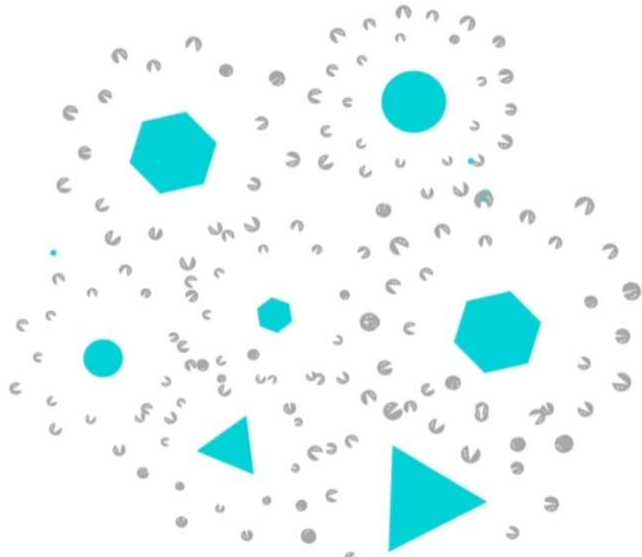
- ▶ Guidance document:

[http://apli1.oecd.org/olis/2007doc.nsf/linkto/env-jm-mono\(2007\)2](http://apli1.oecd.org/olis/2007doc.nsf/linkto/env-jm-mono(2007)2)

From Bob Diderich, OCDE, ENV/EHS

-M. Philippe 16.01.2024

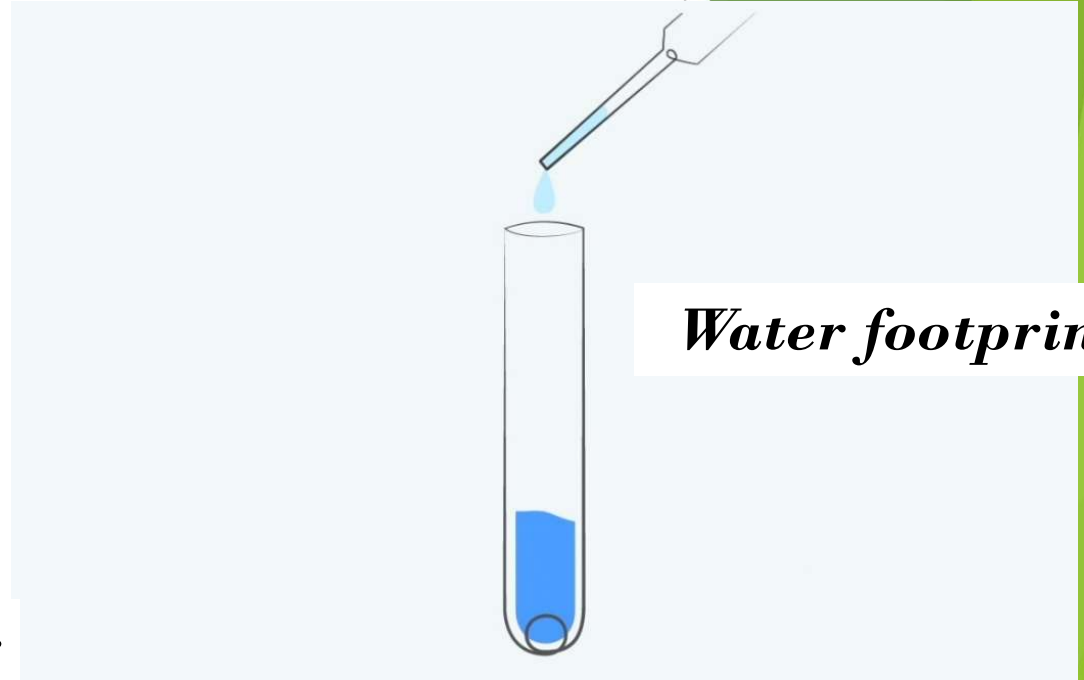
## ***BIODEGRADABILITY AND WATER FOOTPRINT***



### ***Biodegradability***

*Capacity of formula organic RM to be quickly and entirely degraded by microorganisms in the environment*

	<u>Methods</u>
Ready Biodeg.	OECD 301 / 310
Inherent Biodeg.	OECD 302



### ***Water footprint***

*Volume of freshwater required to dilute the formula released down the drain down to no foreseen adverse effect*

### **Measured aquatic toxicity**

<u>Species</u>	<u>Methods</u>
✓ Algae	OECD 201/221
✓ Daphnids	OECD 202/211

## EN PRATIQUE POUR DEVELOPPER UNE **CHIMIE DURABLE**, QUELS SONT LES POINTS ESSENTIELS A PRENDRE EN COMPTE DANS LA FEUILLE DE ROUTE?

- ▶ • Anticiper au plus tôt l'impact (environnemental, toxicologique) du produit final afin de le minimiser ou de rechercher des alternatives:
  - ❖ *Modélisation, méthodes et tests prédictifs, QSAR, Métriques...*
- ▶ • Eco-concevoir des procédés/voies de synthèse à faible impact
  - ❖ *Chimie Verte, Biotechnologies, méthodes physiques...*
- ▶ • Valider ou créer les filières d'approvisionnement durables (à faible impact) économiquement viables
  - ❖ *Utilisation de co-produits, déchets, biomasse, voies circulaires après évaluation des risques...*

EN RESUME:

« **ANTICIPER PAR L'ECOCONCEPTION TOUT AU LONG DU CYCLE DE VIE DU PRODUIT** »



MERCI POUR  
VOTRE  
ATTENTION

***A VOTRE DISPOSITION  
POUR LES ECHANGES***

M. Philippe PhD,  
Consultant in Eco-design, Green Chemistry and Naturalness  
Ex-L'Oréal Fellow  
[michel.philippe7@wanadoo.fr](mailto:michel.philippe7@wanadoo.fr)

M. Philippe 29.09.2023