INSIGHT – Integrated Models for the Development and Assessment of High Impact Chemicals and Materials

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1. Introduction

The INSIGHT project will provide a **novel, integrated framework for mechanistic impact assessment of chemicals and materials**. This multi-layer framework consists of a data graph, a model graph and an impact outcome pathway (IOP) graph that predict the health, environmental, social and economic impacts of chemicals and materials (Fig.1). The three graphs will be systematically interlinked together and used for integrated impact assessment of chemicals and materials for next generation integrated SSbD. Although individual models and data sets for impact assessment exist, they have never been integrated in a network structure. Thus the individual graphs and their integration represent a novel way to approach impact assessment in a mechanistic and holistic way. INSIGHT will save industry money and time in developing and producing chemicals/materials and products derived from them. It will help regulators and policy makers, make informed decision-making that improve safety and sustainability. INSIGHT is fully aligned with the EU principles of safety and sustainability of enabling and emerging technologies of chemicals and materials, as addressed in the EU's Chemical Strategy for Sustainability (2020), in the European Green Deal (2021) and in the Advanced Materials 2030 Initiative (AMI2030). INSIGHT supports the European Green Deal, through which Europe aspires to become the first climate neutral continent by the year 2050. Results from INSIGHT will support policy development in the areas of neutrality, biodiversity protection, public health, and circular economy. INSIGHT is also aligned with the EU's Chemical Strategy for Sustainability (CSS) and will aid the development of a dynamic economy respecting planet Earth as a whole, avoiding harm to humans and the environment. Finally, INSIGHT is funded upon and supports extensively the computational framework being developed within multiple actions including the PARC project, an EU-wide programme that supports chemical risk assessment and risk management.

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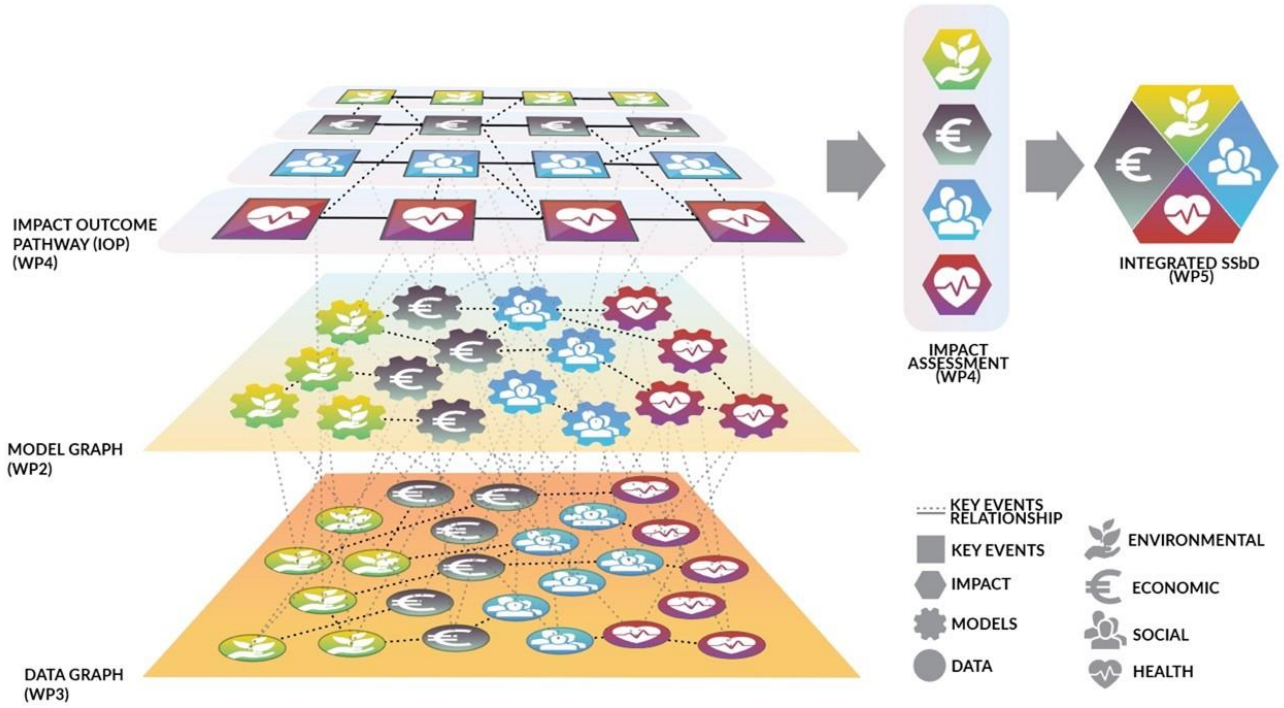

Figure 1: Illustration of the INSIGHT Framework for integrated impact assessment and SSbD.

2. INSIGHT's R&I Objectives

A new era just initiated, in which artificial intelligence and machine learning are creating paradigm shifts in many fields of human activity. Consequently, new functional paradigms of human-AI collaboration are urgently needed. In this scenario, chemical and material development is no exception. Specific challenges including lack of coordination between stakeholders (industry, regulators and academia), limited access to relevant data and lack of method standardisation have thus far hampered the emergence of a comprehensive approach to SSbD. Despite the existence of several frameworks for assessing chemicals and materials throughout their lifecycle, this field remains fragmented, with novel computational approaches disjointed and difficult to access and use. Similarly, FAIR data is necessary for AI-enabled tools, but so far, no clear action has been taken to integrate them from multiple available sources. INSIGHT is designed to drive the innovation towards digitally enabled circular, climate-neutral and sustainable economy by democratising the use of cutting-edge AI-enabled methods to SSbD. Chemical safety is based upon the concept of Integrated Approaches to Testing and Assessment (IATA), where multiple sources of information are used. INSIGHT will expand the IATA concept by developing the next generation Safe and Sustainable by Design (SSbD) procedure in which social, economic, health and environmental impacts are evaluated in a mechanistic and integrated fashion.

Hence, the INSIGHT project aims to:

1. Develop an integrated framework for mechanistic impact assessment based on the novel concept of IOP;
2. Provide curated and user-friendly FAIR data and computational models and workflows that support the development of the next generation SSbD chemicals and materials;

3. Provide open, accessible and interactive guidelines, enabling end users and stakeholders to access and operate the framework.

INSIGHT aims to foster a paradigm shift in the assessment of sustainability and safety of chemicals and materials, from the current fragmented situation towards a holistic and integrated approach. INSIGHT will use the SSbD principles and Life Cycle thinking approach to consider the intrinsic properties of chemicals and materials, production phase, end-user utilisation phase, and functionalities of the product for a comprehensive social, economic, health and environmental impact assessment. Health impacts will be assessed through hazard and risk models, while environmental impacts will be assessed through Life Cycle Impact Assessment (LCIA), following the Product Environmental Footprint methodology. Socio-economic impacts will also be addressed using social-LCA framework and Life Cycle Costing principles.

3. INSIGHT's Policy Alignment

INSIGHT is fully aligned with the EU principles of safety and sustainability of enabling and emerging technologies of chemicals and materials, as addressed in the EU's Chemical Strategy for Sustainability (2020), in the European Green Deal (2021) and in the Advanced Materials 2030 Initiative (AMI2030). INSIGHT supports the European Green Deal, through which Europe aspires to become the first climate neutral continent by the year 2050. Results from INSIGHT will support policy development in the areas of neutrality, biodiversity protection, public health, and circular economy. INSIGHT is also aligned with the EU's Chemical Strategy for Sustainability (CSS) and will aid the development of a dynamic economy respecting planet Earth as a whole, avoiding harm to humans and the environment.

4. INSIGHT's Decision-Support System & GUI

INSIGHT will develop an integrated decision-support system in the form of interactive decision maps. These maps will be multi-level workflows designed for guided decision-making by industrial and regulatory stakeholders and will be adapted to multiple types of SSbD use cases.

The decision maps will also guide the development of the INSIGHT framework GUI (graphical user interface).

Figure 2: Illustration of the decision maps and the INSIGHT Framework GUI.

The GUI will be customisable to suit different user groups' needs and preferences. A Software as a Service (SaaS) option will also be available, hosted on a scalable and secure cloud infrastructure, making it easier for end-users to collaborate and share data with partners and stakeholders, and providing an additional level of convenience and accessibility.