PINK – computational approaches for industry-ready Safe-and-Sustainable-by-Design

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1. Introduction

The PINK project [1] (Provision of Integrated Computational Approaches for Addressing New Markets Goals for the Introduction of Safe-and-Sustainable-by-Design Chemicals and Materials) is funded under the call HORIZON-CL4-2023-RESILIENCE-01-23 - Computational models for the development of safe and sustainable by design chemicals and materials and coordinated by Slovenia-based SME Seven Past Nine d.o.o. It started in January 2024 with a team of 12 beneficiaries, 2 affiliated entities and 2 associated partners and will run for four years.

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2. PINK's objectives

Safe-and-Sustainable-by-Design (SSbD) advanced materials and chemicals (AdMas&Chems) are a central requirement for reaching the ambitious goal of making Europe the first digitally-enabled circular, climate-neutral and sustainable economy. Such new AdMas&Chems need to provide the high functionality required for their advanced applications, whilst simultaneously exhibiting improved safety and sustainability performances that take into account the complete value chain and life cycle, as outlined in the SSbD framework proposed by the EU Joint Research Centre and adopted in the Commission Recommendation of 8 Dec. 2022. To facilitate adoption by industry and, by doing so, foster the twin green and digital transition of Europe's economy, PINK's overarching aim is to produce innovative modelling software and integrated workflows for the development of AdMas&Chems, which are combined into an industry-ready open innovation platform, the PINK In Silico Hub (PINKISH).

3. PINK's tiered approach

PINK takes a holistic approach addressing the needs of industry by solving a multi-objective optimisation problem to improve and balance the four requirement categories functionality, cost-efficiency, safety and sustainability (Figure 1). All five steps of the SSbD Framework (hazard assessment, human health and safety aspects in the production and processing phase, human health and environmental aspects in the final application phase, environmental sustainability assessment, and socio-economic sustainability assessment) are integrated into selection considerations at each stage of the AdMas&Chems development, starting with a limited set of evaluation criteria and rough estimates (low-tier methods) and moving to higher-tier methods in later stages. In this way, confidence in the predictions is continuously improved over multiple design cycles by producing new knowledge on a constantly reduced set of better performing candidates.

PINK combines computational models and a decision support system (DSS) that exploit the combined power of first-principles simulation and pre-existing data, which - in itself - is further improved by advanced artificial intelligence (AI) technology. This requires the integration of tools from different and hitherto independently developed areas (e.g. materials modelling, (nano)safety, life cycle assessment). PINK provides this integration in the form of PINKISH based on an advanced semantic and technical Interoperability Framework, giving access to all information and knowledge, and executing SSbD workflows customisable to (a) the application area of the AdMas&Chems, (b) their safety and sustainability concerns of the existing materials, and (c) the status of the relevant development project (from early design ideas to registration and market entry). Industry readiness of the solution will be guaranteed by improving usability, practicability, user experience, and 'data provenance' documentation and security and by integrating these as important aspects into the development of new modelling software and decision support services. The sequence of implementation of the tools will be customised to real-life needs, to improve existing and new AdMas&Chems by industry partners in the PINK Developmental Case Studies and Industrial Demonstrators.

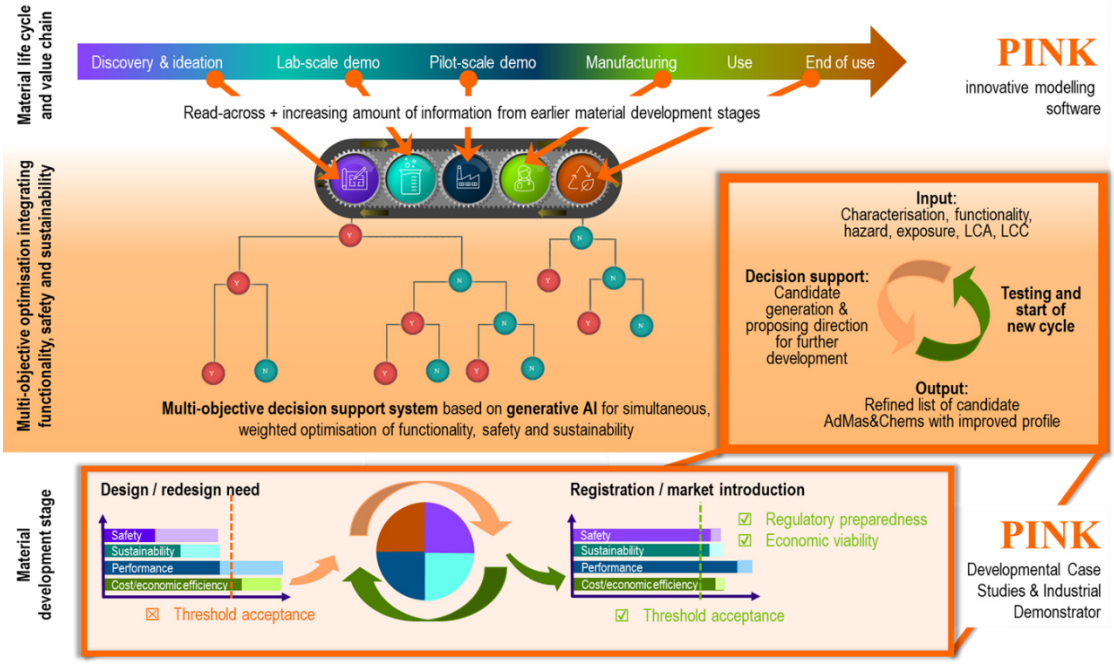

Figure 1: Schematic presentation of the PINK R&I Approach of integrating the SSbD Framework into the development cycle of AdMas&Chems. This will be achieved by solving the multi-objective optimisation problem (middle part) to improve and balance the four requirement categories (i.e. functionality, cost-efficiency, safety and sustainability, lower part) at each stage of the development. Existing data will be integrated and data gaps be filled using innovative modelling and simulation approaches from the complete life cycle and value chain (upper part).

4. Conclusions

PINK's central objectives can be summaries as:

- develop a toolbox of data resources, models and workflows (PINK Services), benefitting from the interoperability and synergy of integrated approaches and provide them as openly accessible software tools and web services;
- build a framework and toolset for technical and semantic interoperability (Interoperability Framework and Infrastructure), based on high FAIRness (findable, accessible, interoperable and reusable) standards essential for information transfer within PINK and enabling re-use by other SSbD workflows or platforms;
- integrate all data and modelling services into the PINKISH platform to facilitate data visualisation, analysis, and the implementation of a comprehensive AI-enabled SSbD decision support workflow; and
- showcase how the computational and digital approaches can boost the innovative capacity of industry and especially SMEs in Developmental Case Studies and Industrial Demonstrators providing real-world stress testing of the provided solutions.

5. References

[1] https://pink-project.eu

6. Acknowledgement

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