Advancing Material and Chemical Development through Innovative Computational Modelling in the PINK Project

Haralambos Sarimveis[1], Steffi Friedrichs[2], Francesca L. Bleken[3], Anna L. Costa[4], Francesco Mercuri[5], Antreas Afantitis[6], Antonino Marvuglia[7], Tommaso Serchi[8], Dario Greco[9], Penny Nymark[10], Martin Himly[11], Karin Wiench[12], Philippe Jacques[13], Iseult Lynch[14], Andreas Karwath[15], Georgios Gkoutos[15], Roland Hischier[16], and Thomas E. Exner[17]

1. Introduction

The PINK project represents a groundbreaking initiative at the forefront of material and chemical innovation. Positioned within the landscape of contemporary scientific research and industry needs, it aims to revolutionise the way advanced materials and chemicals are developed. By harnessing the power of cutting-edge computational modelling techniques and aligning with the principles of Safe-and-Sustainable-by-Design (SSbD), the project seeks to create a computational infrastructure for materials and chemicals that are not only functional but also inherently safer and more sustainable.

[1] School of Chemical Engineering, National Technical University of Athens, Athens, Greece
[2] AcumenIST SRL, Brussels, Belgium
[3] Process Technology, SINTEF AS, Oslo, Norway
[4] Istituto di Scienza, Tecnologia e Sostenibilità per lo Sviluppo dei Materiali Ceramici. Consiglio Nationale Delle Ricerche, Faenza, Italia
[5] Istituto per lo Studio dei Materiali Nanostrutturati (ISMN), Consiglio Nazionale delle Ricerche, Bologna, Italy
[6] Novamechanics Limited, Nicosia, Cyprus
[7] Environmental Sustainability Assessment and Circularity Unit, Luxembourg Institute of Science and Technology, 4362 Esch-sur-Alzette, Luxembourg
[8] Environmental Research and Innovation, Luxembourg Institute of Science and Technology, 4362 Esch-sur-Alzette, Luxembourg
[9] Division of Pharmaceutical Biosciences, University of Helsinki, Helsinki, Finland
[10] Institute of Environmental Medicine, Karolinska Institutet, Stockholm, Sweden
[11] Department of Biosciences & Medical Biology, Paris Lodron Universität Salzburg, Salzburg, Austria
[12] BASF SE, Ludwigshafen, Germany
[13] Energy Materials Industrial Research Initiative AISBL, Brussels, Belgium
[14] School of Geography, Earth and Environmental Sciences, University of Birmingham, Birmingham, UK
[15] Centre for Health Data Science, University of Birmingham, Birmingham, UK
[16] Advancing Life Cycle Assessment, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, Switzerland
[17] Seven Past Nine d.o.o., Cerknica, Slovenia, thomas.exner@sevenpastnine.com

2. PINK Modelling and Decision Support Framework

Central to the PINK Modelling Framework is the harmonization of diverse data models and software tools, aimed at addressing complex multi-objective optimization challenges. These challenges encompass balancing functionality, cost-efficiency, safety, and sustainability in material and chemical development. In line with the recently proposed SSbD framework, a detailed library of data analytics and machine learning models is under development. This library is crafted to predict the functionalities and impacts of materials and chemicals across their entire lifecycle, encompassing all stages from production through to disposal.

A crucial element of the PINK project's modelling work is data-driven and AI-based methodologies, such as QSAR and QSPR models, which are employed to predict material properties and impacts. Complementing this, multi-scale modelling is offering essential insights into material properties across various scales, from atomic to macroscopic. Incorporating life-cycle assessment (LCA) methods further enriches the project, enabling an evaluation of the environmental impact of materials across their entire life cycle. The integration of both exploratory and prospective LCA approaches allows understanding of sustainability impacts at various developmental stages. Moreover, the project will incorporate advanced methods in toxicogenomics, which involves using omics technologies to understand the molecular mechanisms underlying the toxicity of substances. Mechanistic models, notably Physiologically Based Kinetic (PBK) models, will play a pivotal role in risk assessment and biokinetics simulations.

For the development of safe production processes, data-driven multi-objective optimization algorithms like Bayesian optimization will be utilised. These techniques help in identifying optimal conditions in production processes, balancing factors like yield, environmental impact, and product consistency. Generative learning and explainable AI are also key components of the project. Generative models will be used to explore vast chemical spaces and propose novel structures, thus driving innovation in material and chemicals design.

The PINK project's decision-support strategy is built on an iterative approach, which effectively narrows down potential material and chemical candidates through successive iterations. In each iteration, a vast array of candidates is evaluated and filtered based on a multitude of factors, including functionality, safety, sustainability, and cost-efficiency. As the process advances, the number of candidates reduces, and the focus intensifies on those with the most promising profiles. Explainable AI will ensure that the decision-making process in the material development is transparent and understandable, crucial for gaining trust and acceptance in the industry.

3. Conclusions

The PINK project aims to establish a new benchmark in material and chemical development by integrating diverse, advanced modelling methods into a unified and coherent framework. It aligns the goals of enhanced functionality with environmental responsibility and safety, paving the way for a more efficient and sustainable approach to material and chemical innovation.

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