Towards a Generalized Scale-Up Methodology in Prospective LCA: Enabling the SSbD Assessment (a status update)

Marc Majó, Roland Hischier
Empa, Technology & Society Laboratory, St. Gallen, Switzerland

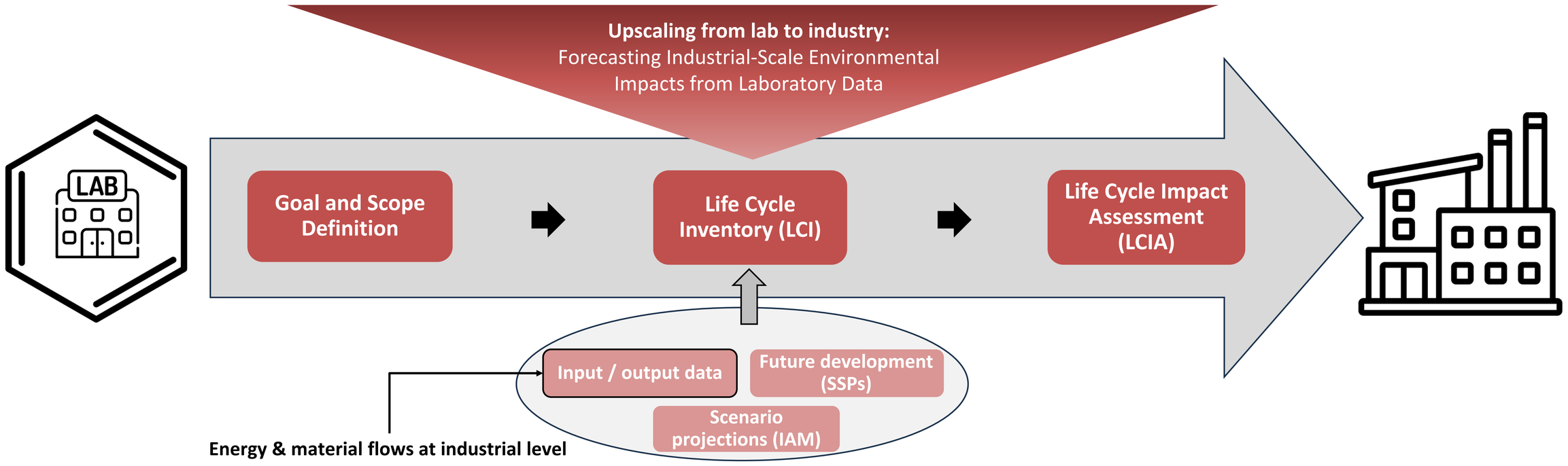
Empa
Materials Science and Technology

Context

Assessing the sustainability of **emerging materials** requires shifting the focus toward a higher TRL by building an **industrial-scale Life Cycle Inventory (LCI)**. However, for novel substances, environmental data are limited and often non-representative of industrial conditions. Having a proper upscaled LCI will enable accurate calculation of future impacts through **Prospective Life Cycle Assessment (pLCA)**

	Production energy (MJ/m³)	Deviation
Lab-Scale → Industrial benchmark	204532	+2414%
Upscaling methodology → Industrial benchmark	12209	+50%
Industrial benchmark	8139	-

Comparison of production energy of an aerogel: lab scale vs industrial benchmark. *Dowson et al. 2012*

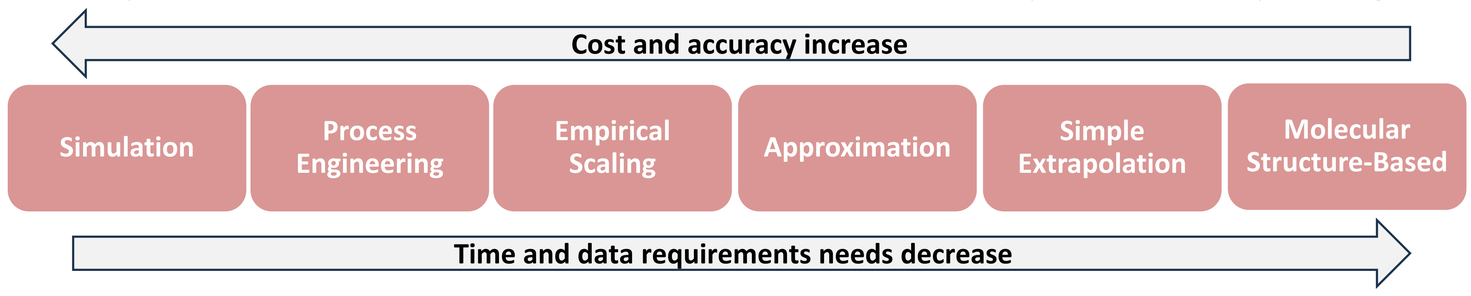


The lack of a generalized approach to translate laboratory data into realistic industrial inventories within pLCA leads to limited comparability and a resource- and time-intensive implementation. This work develops **generalized, sector-tailored guidelines** that identify **minimum data requirements, critical non-linear upscaling parameters, and methodological pathways for biochemical, petrochemical, and pharmaceutical** systems to support early-stage assessments under the Safe and Sustainable by Design (SSbD) framework.

Our approach

1 Identification of Upscaling Procedures and Data Requirements

A number of methods and strategies for scale-up have been proposed and applied across literature. A key limitation often is the lack of complete datasets with detailed mass and energy balances, precise yield reactions, or accurate steps or processes at larger scale. An analysis of different methodologies with advantages, limitations and data requirements has been conducted. These outcomes will be reported in an (upcoming) scientific paper.



2 Identification of general and specific parameters to be included

General upscaling parameters

- $Re = \frac{\rho u D}{\mu}$ — **Flow regime**
- $Pe = \frac{uD}{D_m}$ — **Convective transport**
- $Nu = \frac{hD}{K}$ — **Heat transfer**
- $Da = \frac{kL}{u}$ — **Reaction time**
- $Sh = \frac{k_m D_p}{D_m}$ — **Mass transfer**

Sector-specific parameters

Petrochemical

Refinery complexity and Energy integration:

- Refinery complexity index (NCI)
- Energy integration and heat recovery networks (continuous reaction)

Biochemical

Biological and Hydrodynamic Sensitivities:

- Constant $k_L a$ for constant O_2 rate
- Constant tip speed for shear-sensitive systems
- Constant mixing time for environmental homogeneity

Pharmaceutical

Purity, Control, and Facility Energy Demand:

- Energy input for HVAC and clean utilities
- Crystallization and drying processes
- Formulation and API production

3 Definition of core upscaling parameters governing material and energy flows across scales

4 Development of standard procedures to convert laboratory data into representative industrial LCIs

Prepare foundation for data-driven prediction, enabling integration of AI & process simulation tools for automated LCI generation

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marc.majo@empa.ch

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