Toward a Generalized Scale-Up Framework in Prospective Life Cycle Assessment

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1. Introduction

Prospective Life Cycle Assessment (pLCA) is increasingly applied to evaluate emerging chemicals and materials before industrial product exist. However, most early-stage assessments rely on laboratory data that do not reflect industrial operating conditions. Laboratory experiments typically show disproportionately high electricity demand, excess solvent and reagent use, limited separation efficiency, and batch-driven losses that distort environmental profiles when directly scaled to industrial systems. These discrepancies complicate model extrapolation and hinder the reliability and comparability of prospective assessments.

Current challenges in this topic are (i) the absence of a generalised procedure for translating laboratory-scale material and energy flows into industrial-scale life cycle inventories, and (ii) a need for tools and/or frameworks, capable to provide a clear and robust industrial level calculations, especially for those mechanism connected with heat-mass transfer behavior, equipment efficiency and utility demand. Hence, a systematic approach is needed to define how early-stage data should be interpreted, adjusted, and supplemented to yield realistic industrial representations [1]. The present analysis focus on three specific sectors: biochemical, petrochemical and pharmaceuticals, each characterised by sector-specific scaling-up challeges – ranging from high energy petrochemical systems over biological limitations associated to biochemical processes to high-purity separations and HVAC utilities in pharmaceutical production. The objective here is to consolidate existing pLCA and scaling-up knowledge (applied to the LCA) to identify the scaling drivers responsible for environmental impact in these three sectors, and develop a generalized approach to guide LCA at early stages of development.

2. Critical-point analysis: Identification of key scaling drivers

An analysis of laboratory versus industrial operation reveals that several flows exhibit strong non-linearities upon scale-up. Different case studies were explored and five categories have been listed in Figure 1.

ASPECT	LABORATORY SCALE	→	INDUSTRIAL SCALE
Energy	High specific energy: short cycles, no recovery	Scale via A/V, apply continuous-operation assumptions depending on sector, add heat recovery	Integrated networks, reduced energy per FU
Material	Excess solvent/catalyst, single-phase use	Replace excess with optimized stoichiometry, apply recovery efficiencies	Closed-loop recovery, optimized dosing
Waste	Unmanaged, small streams	Add scrubbers, wastewater treatment off-gas capture	Managed waste systems, controlled emissions
Infrastructure	Negligible (underutilized equipment)	Include reactors, utilities, clean-in-place, distillation columns	Infrastructure dominates embodied impacts
Data	Precise but not operationally representative	Combine lab data with simulation and proxy analogues	Continuous operational datasets (adapted to sector)

Figure 1: Considerations for energy and material flows at lab scale and industrial scale [2][3].

In general, laboratory systems show high electricity use, elevated reagent and solvent consumption, and unmanaged wastes due to poor insulation, intermittent operation, and single-pass practices. Their data reflect early experimental conditions with negligible infrastructure effects.

Industrial systems, on the other hand, optimize these flows through continuous operation, heat recovery, solvent and catalyst recycling, and dedicated emission controls. Material impacts grow with throughput and optimized stoichiometry, while waste and infrastructure contributions decrease as unit operations expand due to optimization lines, yet remaining comparatively less relevant to the overall impacts. Data shift toward aggregated operational measurements and model-based estimates.

Recognising these scale-dependent drivers clarifies which parameters require adjustment when extrapolating laboratory data and underpins the generalised upscaling procedure.

3. Step-by-step upscaling procedure

3.1. Step 1 – General upscaling aspects

In a first step, generalized upscaling aspects are considered. They focus on the main unit operations that dominate material and energy demand: heating, cooling, drying and solvent recovery. This include the selection of appropiate boilers or furnaces, heat-transfer media, cooling technologies; industrial drying equipments; and solvent-recovery units (through distillation or membrane separations). For this, our procedure is supported by a tool capable of calculating the amount of energy and fuel consumed based on data available at low Technology Readiness Levels (TRL), enabling the creation of different scenarios based on fuel type, operating temperature, and technology choices. Data are then organised into minimum datasets covering stoichiometry, yields, solvent and reagent flows, mixing, thermal loads and waste streams, forming the basis for consistent scaling up.

3.2. Step 2 – Sector-specific aspects

After the above general aspects, sector-specific mechanisms are then explored in the 2nd step:

Petrochemical systems rely on thermodynamic integration, heat-exchange performance and dimensionless number to capture flow, heat and mass transfer. A refinery-complexity index indicates integration potential and separation intensity.

Biochemical systems scale via the dominant limiting mechanism (oxygen transfer, shear sensitivity, circulation or CO_2 removal) while accounting for non-Newtonian behaviour. Parameters such as k_La, power density and hydrodynamic similarity translate lab kinetics to industrial reactors.

Pharmaceutical systems are driven by high-purity operations. Crystallisation, filtration, solvent purification and drying dominate, while HVAC and solvent-intensive API synthesis strongly influence utilities and infrastructure.

Incorporating these sectoral mechanisms aligns the general framework with the operational, thermodynamic and regulatory constraints of each domain.

4. Conclusions

Our study proposes a unified, step-wise procedure for converting laboratory data into representative industrial LCIs. It integrates critical scaling drivers, a general upscaling strategy and sector-specific refinements. By combining engineering principles with thermodynamic, mass-transfer and sector-dependent constraints, the framework strengthens robustness and transparency in early-stage pLCA. It corrects systematic distortions in laboratory inventories and offers a structured path to generate realistic industrial scenarios under limited information.

5. References

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