Toward a Generalized Scale-Up Methodology for chemical/materials production in Prospective LCA

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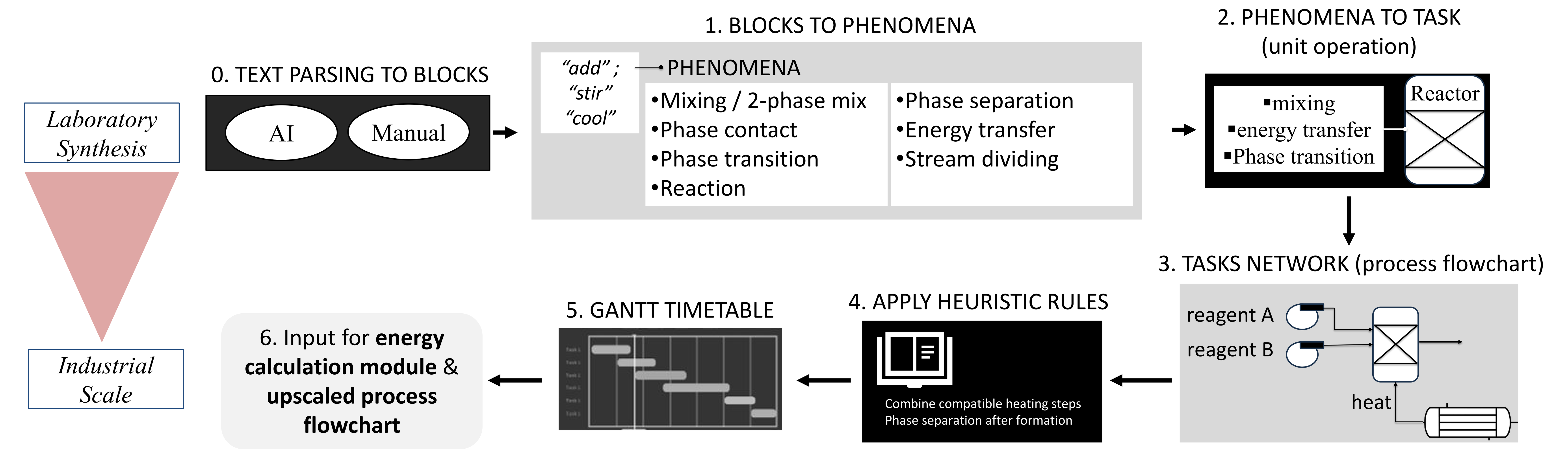
Context

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. To address this gap, the proposed guideline translates laboratory synthesis narratives into scalable industrial process flowsheets using a **phenomena-based approach** that integrates **process engineering knowledge** for unit operation selection, **heuristic rules**, and **process optimization** through scheduling analysis. The framework aims to support robust early-stage assessments within the **Safe and Sustainable by Design (SSbD)** framework.

Methodological approach

Guideline from lab protocol to industrial flowsheet



Illustrative Example

Upscaling octocrylene synthesis to industrial level

Lab synthesis narrative: *"To a round-bottom flask equipped with a stirrer and coupled with a condenser, add 2-ethylhexyl cyanoacetate, benzophenone, the chosen solvent (cyclohexane), and the catalyst (NH_4OAc). Stir and reflux (85 – 145 °C), the formed water needs to be removed to drive the equilibrium towards the product. Monitor until benzophenone concentration ceases to decrease. Cool to RT, wash the crude with water and brine, and dry over anhydrous $MgSO_4$ or Na_2SO_4. Filter and purify in a distillatory to obtain the final octocrylene."* → ***Upscaling to industrial production: 750 t/year***

Protocol blocks and phenomena *(step 0 to 1)*

Block	Dominant phenomena
B1: Charge	2phM(LS)
B2: Heat to reflux	M=ES(H)=PT(LS)
B3: Reflux reaction	M=2phM=R(V)=ES(H)=PC(VL)=PT(VL)
B4: Cool	M=ES(C)
B5: Aqueous wash	M=PT(MLL)=PS(LL)
B6: Brine wash	M=PT(MLL)=PS(LL)
B7: Drying (chemical)	M=PC(LS)=PS(LS)
B8: Solvent removal	M=ES(H)=PT(VL)=PS(VL)
B9: Vacuum distillation	M=ES(H)=PT(VL)=PS(VL)

M = Mixing
2phM = Two-phase mixing
ES = Energy supply
PC = Phase contact
PT = Phase transition
PS = Phase separation
Liquid (L), vapour (V), solid (S), heating (H), cooling (C), component affinity liquid-liquid (MLL)

Tasks and selected Unit Operation *(step 2)*

Tasks	Selected UO
T1: Reaction (B1,2,3,4)	Semi-batch stirred reactor + reflux condenser + side decanter
T2: Wash (H_2O+Brine); (B5,6)	Two-stage mixer
T3: Drying (B7)	Fixed-bed molecular siever
T4: Solvent removal (B8)	Thin-film evaporator
T5: Distillation (B9)	Short-path distillation
T6: Catalyst removal (B5,6)	Combined into T2
T7: Vent abatement	Vent condenser + activated carbon polish

Upscaled units and Heuristic knowledge *(step 3 to 4)*

Units	Main activity	Heuristic rules
U1: Feed-tank (T1)	Charge to U2	For equilibrium reaction, water needs to be directly removed – reflux condenser and decanter needs to be coupled to the reactor.
U2: Reactor (T1)	18-24h Reactor+Dean-stark	
U3: Mixer-settler (T2)	Aqueous+brine wash	Distillation unsuitable due to phase partitioning. Water/brine countercurrent washing minimizes solvent use.
U4: Sieve drying column (T3)	Organic drying	Molecular sieve separation is valid since the size ratio of compounds exceeds 2. Avoid singe-use dissecans reduce waste.
U5: Thin-film evaporator (T4)	Cyclohexane removal, recycled to U1	With 1.75 boiling-point ratio and heat sensitivity of products, cyclohexane is recycled while octocrylene is separated preserving its quality
U6: Short-path distillation (T5)	Final purification	Short-path distillation minimizes residence time and thermal exposure
U7: Vent condenser (T7)	VOC compliance	Industrial VOC rules require vent abatement
U8: Cyclohexane recovery distillator	Solvent recycle to U1	Recycling streams included for cyclohexane
U9: Brine and WWT neutralization unit	Aq waste discharge	Waste water treatment (WWT) routes for discharge

Input for energy calculation module

Scheduling *(step 5)*: Cycle-time analysis, bottle neck identification and time reduction (parallelization)

Upscaled industrial flowsheet

Prepare foundation for data-driven prediction, enabling a guided upscaling and energy calculation for automated LCI generation

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