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Up-scaling methods used in ex-ante life cycle assessment of emerging technologies: a review

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1 Results

1.1 Projected data estimation

1.1.1 Process simulation

A potential industrial-scale model of a new technology can be simulated using process simulation. In this review paper, process simulation is defined as a data estimation method that involves the use of simulation software and databases. Process simulation starts with the process design to prepare simulation processing flowsheets. The process design is done following a hierarchical design strategy based on heuristics and experience (Fernández-Dacosta et al. 2015). During the process design, suitable mathematical models are selected from the simulation software library and process operation parameters are used as inputs to the models. The process operation parameters can be obtained from lab or pilot-plant experiments or from literature. When the processing flowsheets are ready, simulation software is used to calculate the results for energy flows, material flows and environmental interventions. Table 1 shows which simulation software was used in the reviewed ex-ante LCA studies.

Table 1 Studies that performed data estimation using process simulation

Study	Technology	Simulation software
Cossutta et al. (2017)	Graphene production	SuperPro Designer (Intelligen Inc. n.d.).
Fernández-Dacosta et al. (2015)	Microbial community-based polyhydroxyalkanoates (PHAs) production from wastewater	Aspen Plus (Aspentech n.d.)
González-García et al. (2018a)	Production of bio-succinic acid from apple pomace[a]	Aspen Plus (Aspentech n.d.)
Mazzoni et al. (2019)	Biorefining of ethanol	Aspen Plus (Aspentech n.d.)
Rinaldi et al. (2015)	Pyrolysis-gasification of automotive shredder residue	CHEMKIN (Reaction Design n.d.) 2. FLUENT (ANSYS n.d.) 3. Aspen Plus (Aspentech n.d.) 4. CHEMCAD (Chemstations n.d.)
Khojasteh Salkuyeh et al. (2017)	Syngas chemical looping (SCL) and chemical looping reforming (CLR)	Aspen Plus (Aspentech n.d.)

[a] The authors did manual calculations to estimate data, however, they used process simulation in the specific design of the equipment

1.1.2 Manual calculations

Manual calculations can be used to calculate energy and materials inputs and outputs and environmental interventions such as emissions and resource use. Manual calculations are defined as a data estimation method that involves calculations done manually, e.g. using mathematical and physical equations, stoichiometry, scaling factors, etc.

Basic mathematical and physical equations can be used to calculate data manually. Arvidsson and Molander (2017), who up-scaled epitaxial graphene production from lab and pilot scale to industrial scale, calculated the energy for heating silicon carbide (SiC) wafer using heat equation:

$$E = c_p m \Delta T \qquad (1)$$

where:
E – required heat for the temperature change
c_p – heat capacity of SiC
m – mass of the SiC wafer
ΔT – temperature change

Arvidson and Molander (2017) also calculated the mass of SiC required for graphene production. First, they made assumptions regarding the thickness of the SiC wafers at industrial scale. For the worst-case scenario, they assumed that the wafer thickness would be the same as at pilot scale, 500 µm. For the best-case scenario, they assumed that increased production of epitaxial graphene would spur the development of thinner SiC wafers so that a thickness of 50 µm would be obtained. Using these thickness values, they calculated the mass of SiC required to make the wafers by using the following equation:

$$m = \frac{N\pi\left(\frac{d}{2}\right)\text{^}(2)hp}{N\pi(\frac{d}{2})\text{^}2} \qquad (2)$$

where:
h - thickness of the wafer
p – density of SiC
N – number of wafers per batch
d- wafer diameter

Mattick et al. (2015) calculated the inputs and outputs of materials for in vitro biomass production for cultured meat, e.g. inputs of nutrients (glucose and glutamine), and outputs of byproducts (lactate, alanine, ammonia). They made assumptions regarding some cell culture model parameters (e.g. the bioreactor volume, a specific growth rate of cells during proliferation), obtained the nutrient uptake and byproduct formation rates for cells from literature and used them to calculate the inputs and outputs of materials using physical equations.

Muñoz et al. (2019) up-scaled solar-assisted heat pump (SHP) from pilot-scale to industrial scale. They calculated the input of energy for the operation of equipment in SHP: individual equipment for SHP was redimensioned and/or the number of units was increased. Based on up-scaled equipment, the cooling and heating capacity of SHP was approximated. These capacity values were used to estimate energy inputs. Muñoz et al. (2019) calculated the total thermal energy recovered based on experimental pilot-plant data and approximated energy input to SHP: knowing how much energy could be recovered per a certain volume of wastewater at a pilot-plant, they approximated the potential thermal energy recovery from wastewater at an up-scaled industrial plant. The contribution of solar energy was deduced from the potential energy production by the up-scaled SHP. Then the contributions of SHP (energy for the operation of equipment in SHP) and thermal energy recovery were summed.

Cuéllar-Franca et al. (2016) up-scaled the production of ionic liquid for CO_2 capture from lab scale to industrial scale. They calculated the heating and cooling energies required by reactors for the production of the ionic liquid. First, they calculated the theoretical energy based on the heat formation values of reactants and products and then scaled it up by multiplying it with empirical factors that take energy losses into account. First, they calculated theoretical energy using the heat of formation of reactants and products and then scaled it up by multiplying by empirical factors that take into account energy losses. The authors reported that they did not estimate other energy requirements (e.g. energy consumption for pumping and separation rather than heating and cooling energy). The authors justified this by stating that it was unknown which unit operations might be required in a future industrial scale process and what their capacity and configuration could be. However, they checked the effects of this assumption in the sensitivity and uncertainty analyses.

Mass balance calculations can be used for calculations of material inputs and outputs and environmental interventions. Cuéllar-Franca et al. (2016) estimated materials inputs and outputs for the industrial-scale production of ionic liquid, using the stoichiometric relationships for chemical reactions, taking into account the yields or conversions found in literature for each chemical reaction. Piccinno et al. (2018) calculated H_2O and CO_2 emissions of burned acetone. Muñoz et al. (2019) calculated the outputs of emissions and sludge for SBBGR WWTP using the WW LCI model (Kalbar et al. 2018; Muñoz et al. 2017). This model is programmed in an Excel spreadsheet and is based on stoichiometry and mass balance calculations using empirical relationships of parameters in wastewater treatment.

Linear scaling can be used in up-scaling to obtain material inputs and outputs. Arvidsson and Molander (2017) used linear scaling assuming that the electricity consumption for graphene production at industrial scale would be the same as at pilot scale. Piccinno et al. (2018) scaled the input of enzymes for the enzymatic treatment of carrot waste linearly from lab scale to industrial scale. Sampaio et al. (2017) assumed that the amount of reagents and effluent loads applied in each unit process in the gelatin production increases linearly from the laboratory to the pilot scale.

Piccinno et al. (2016) introduced a framework for up-scaling chemical processes. In this framework, calculation procedures, equations, average values and estimations are included to estimate energy and material inputs and outputs and environmental interventions. This framework was used in some case studies (González-García et al. 2018a; González-García et. al. 2018b; Piccinno et al. 2018).

1.1.3 Molecular Structure Models

Molecular Structure Models (MSMs) can be used for data estimation for up-scaling chemical technologies. MSMs are based on neural networks (Hornik et al. 1989) and can calculate key LCI parameters and impact results using the molecular structure of a chemical (Wernet et al. 2009). The literature search for the present review identified one ex-ante LCA study applying MSMs: Mazzoni et al. (2019) used the Finechem Tool (ETH Zurich n.d.) to estimate resource use and environmental impacts for the production of a catalyst that is used in the biorefining of ethanol from wine waste.

1.1.4 Use of proxy

Some studies used proxies as a data estimation method in the up-scaling of unit processes of a new technology. For example, Villares et al. (2016) up-scaled bioleaching of PCB from lab scale to pilot scale. They up-scaled the laboratory shaker flask platform, where bioleaching was taking place, using a set-up of 12 continuous stirred tank reactors (CSTRs) with a volume of 1,625 m^3. This set-up was derived from a modelled integrated plant for the purification and recovery of metals from low grade ores. The stirring energy was calculated assuming that bioleaching took place at these tank reactors.

Mattick et al. (2015) up-scaled the *in vitro* biomass production for cultured meat from lab scale to industrial scale. They modelled the bioreactor configuration based on a large-scale pharmaceutical manufacturing plant, which houses six 15,000 L stirred tank reactors. They calculated the energy required for the biomass cultivation (e.g. the energy required for heating the water, for agitation, and for aeration) using the parameters of those stirred tank reactors.

Muñoz et al. (2019) up-scaled a sequencing batch biofilter granular reactor (SBBGR) and wastewater treatment plant (WWTP) from pilot scale to industrial scale. They assumed that electricity consumption for SBBGR and WWTP would be the same as that of a similar industrial plant. Muñoz et al. (2019) calculated the material inputs for an up-scaled SBBGR WWTP: they first found the value for polyelectrolyte dosage in sludge dry mass in literature. Then they calculated the input of polyelectrolyte to an up-scaled SBBGR WWTP using this value and the mass of potential sludge produced in the up-scaled SBBGR WWTP.

Schulze et al. (2018) up-scaled electrolysis for the extraction of rare earth metals from scrap NdFeB. They found the ranges of electricity and materials consumption of electrolysis in literature and used those ranges to model the electricity and materials inputs of the up-scaled technology.

Sampaio et al. (2017) up-scaled the production of gelatin from tilapia residues from lab scale to pilot scale. The authors developed a table reporting on the equipment used in lab processes and corresponding pilot-scale processes with similar functions for the processes for production of gelatin from tilapia residues (e.g. cutting, hydrolysis, neutralization, washing, extraction, deodorization and demineralization, drying, and milling). The energy required by the pilot-scale machines was calculated as the product of power (kW) and operation time (minutes or hours) of each machine divided by that machine's full capacity. The power, operation times and capacity values of pilot-scale machines were obtained from online catalogs of food production machinery. The machines' loss of energy during the extraction and drying processes was calculated based on the efficiencies found in literature.

Salas et al. (2018) followed the same approach as Sampaio et al. (2017) in the up-scaling of energy inputs. They up-scaled the production of geopolymer concrete from lab scale to industrial scale. At the

laboratory, the production of the geopolymer concrete involves mixing of cement pastes and mortars using a small mixer and the manual preparation of geopolymer concrete specimens in a wooden mold. The authors assumed that a concrete pan mixer and a vibrating block making machine would be used at industrial scale instead of the small mixer and manual preparation of concrete specimens. They selected suitable commercialized machines and calculated the electricity consumption based on their technical specifications and operation times.

Simon et al. (2016) up-scaled the production of nanofibers for lithium iron phosphate cathode applications. They calculated the energy consumption of electrospinning subprocesses using the load factors and minimum and maximum power requirements of similar industrial processes. The data originated from the machine developers. Simon et al. (2016) used literature data to model emissions from the pyrolysis gas treatment process.

Villares et al. (2016) up-scaled metal recovery from printed circuit board (PCB) using bioleaching from lab scale to pilot scale. The steps for the preparation of bioleaching of PCB were manual cutting, crushing and sieving of PCB. In order to up-scale these lab processes, the authors replaced them by one industrial shredding process adapted from ecoinvent v2.2. This ecoinvent dataset included mechanical treatment infrastructure, energy consumption, emissions to air, and an estimation of the efforts for transportation.

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