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From laboratory to industrial scale: a scale-up framework for chemical processes in life cycle assessment studies

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ABSTRACT

Life cycle assessments (LCA) of an early research state reaction process only have laboratory experiments data available. While this is helpful in understanding the laboratory process from an environmental perspective, it gives only limited indication on the possible environmental impact of that same material or process at industrial production. Therefore, a comparative LCA study with materials that are already produced at industrial scales is not very meaningful. The scale-up of chemical processes is not such a trivial process and requires a certain understanding of the involved steps. In this paper, we elaborated a framework that helps to scale up chemical production processes for LCA studies when only data from laboratory experiments are available. Focusing on heated liquid phase batch reactions, we identified and simplified the most important calculations for the reaction step's energy use as well as for certain purification and isolation steps. For other LCA in- and output values, we provide estimations and important qualitative considerations to be able to perform such a scale-up study. Being an engineering-based approach mainly, it does not include systematically collected empirical data which would give a better picture about the uncertainty. However, it is a first approach to predict the environmental impact for certain chemical processes at an industrial production already during early laboratory research stage. It is designed to be used by LCA practitioners with limited knowledge in the field of chemistry or chemical engineering and help to perform such a scale-up based on a logical and systematic procedure.

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1. Introduction

The sustainability dimension – at the earliest stage of development – is increasingly a demand in research projects. While new materials are being developed at laboratory scale, one task often comprises to prove already in this very early stage their "sustainability" compared to existing materials. Life cycle assessment (LCA), being a widely used and standardized tool to evaluate the environmental impact of a product, process or service, is considered an ideal instrument to evaluate said dimension. Many research projects, however, provide lab-scale data only, which frequently results in a much higher impact when comparing with commercially available materials. Optimized process and scaling effects of the latter result in advantageous material and energy efficiencies. This comparison is therefore not realistically representing the potential of the developed material or process. A scale-up allowing the comparison with competing technologies at the commercial scale, can therefore significantly improve the environmental assessment.

Performing an LCA of any existing process – where relevant in- and output data can be obtained by measurements – is straightforward, however, this task becomes much more difficult when data for a process that will occur in the future is needed. This limits the data quality to the accuracy of predicting future events. Changes in technology, regulations, availability of materials, prices etc. can result in major economic and environmental changes. This inherent unpredictability makes it extremely difficult to simulate the results of a process at an industrial scale, although it is still under development in the laboratory. Up to now, only few studies that focus on scale-up of LCA data are available. Caduff et al. (2011) examined different energy equipment and established scaling laws based on empirical data. Using wind turbines as a case study, they also differentiated between learning and scaling effects by comparing empirical data to theoretical engineering based values (Caduff et al., 2012).

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In the field of chemical engineering, scale-up is a decisive and integral part. Countless literature has been dedicated to this area. Normally, once a process has been proved and optimized in the laboratory scale, the upscaling consists of several steps before the actual plant is built. The construction of a mini plant is followed by a pilot plant to confirm all the processes and measure data simulating the industrial scale process. Hereby, dimensional analysis is a useful and established technique. Hence, the practical scale-up of chemical processes is a complicated, long and case specific procedure where detailed knowledge of chemical engineering is required. The wide knowledge about scale-up of chemical process has not yet been translated into an approach that enables LCA practitioners to scale-up from lab data of the production of new materials.

LCA has been used for the evaluation of chemical processes and its applicability in this area has been assessed (Burgess and Brennan, 2001; Kralisch et al., 2014; Muñoz Ortiz, 2006). To estimate the LCA results of chemicals without the knowledge of the production process, one approach is to predict inventory data and the result of certain impact categories of chemicals solely based on the molecular structure of the target chemical (Wernet et al., 2008, 2009). For the scale-up of chemical processes, Shibasaki et al. (2007) and Shibasaki (2009) proposed a method to scale up chemical processes from a pilot plant to a commercial scale based on the obtained LCA results of the smaller scale. However, this method requires an LCA of a pilot plant and expert knowledge or estimates on how the process will behave (e.g. change of material and energy efficiencies) at the larger scale. Furthermore, the existence of a pilot plant means that the development is already at an advanced stage as it tries to simulate a large-scale process by using similar apparatus and connecting all the steps.

Yet, this study starts on the laboratory scale and provides a procedure on how to simulate an industrial scale production with the available data not requiring knowledge about the behavior at the large scale. In the laboratory, the various steps are normally not directly linked to each other and the type of vessels and equipment used are not comparable to the reactors and machineries of a commercial plant. Hence, an extrapolation from the LCI data of the lab scale does not seem reasonable. Instead, all involved steps should be scaled up singularly by modeling an appropriate plant. To our knowledge, there is no general procedure to scale-up laboratory scale chemical processes to an industrial production. In this paper, we propose an engineering based scale-up procedure to simulate processes and perform LCA studies at a commercial scale with the use of a lab protocol, a publication or patent document only. The goal is to fill a gap by providing this framework on how chemical lab processes can be scaled up for LCA purposes obtaining results that reflect industrial productions.

2. Scale-up procedure

The scale-up framework follows a five-step procedure (Fig. 1). Starting point (1) is a lab protocol that is obtained from the lab experiments directly, a publication or a patent document. This lab protocol should document all the steps and quantities used on the laboratory scale. This information is then used to (2) design a simple plant flow diagram. Such a diagram should include all the steps involved as well as the scale, reactors, apparatus and main equipment. For this purpose, Table 1 can be used as a guidance on how to design the simple plant flow diagram based on the scale-up procedure. In the next step, each individual process step (3) in this plant flow diagram is scaled up according to the procedure of this framework. The (4) linkage and consolidation of the in- and output data of all the involved process steps is then included. This consists mainly of inter-process heat and material recycling as well as the contribution of the plant's infrastructure. All the obtained results are used in the concluding step to (5) perform the LCA.

The overall goal of the developed scale-up framework is to obtain, from an LCA perspective, logically and systematically compiled data, allowing a simulation of the process at a larger scale. It is not the emphasis of the framework to analyze in detail the applicability of the process at a larger scale from a technical perspective. In view of the overall goal, several simplifications had to be made for the sake of the practicality of the suggested framework.

The present paper emphasizes on liquid phase batch reactions including eventual, subsequent purification and isolation steps. Those types of processes are very common in chemical lab research. Being mainly an engineering based scaling, tailored to the needs of an LCA study, the description contains formulas to calculate values, estimates based on average data (from literature as well as experts) and case specific considerations that are relevant for an LCA study. All presented equations are explained and generic values are listed as suggestions. The adaption of the values is possible based on the accuracy of the data of a specific case. Moreover, further considerations are included to support reasonable choices for the scale-up calculations of the process.

Different chemical engineering books were consulted to derive the appropriate equations and calculations as well as to obtain average values (Albright, 2009; Perry and Green, 2008; Takata and Umeda, 2007; Thirumaleshwar, 2009; Ullmann, 2005; Vauck and Müller, 2000). All these calculations have been adapted and simplified to the necessities of a scale-up in the context of an LCA study. For certain steps, average data of processes and/or equipment derived from literature and product information were used. Such information was further complemented by expert experience and estimations.

A liquid phase batch process normally takes place in a batch reactor under stirring and, where necessary, heating or cooling. It is a discontinuous process where the reactor is filled with the feed and only voided after the reaction has taken place. In a continuous process in contrast, the reaction vessel is being fed and voided on a constant flow without interruption. Batch processes are more suited for complex reactions. As a simplification, most reactions that are performed in a small laboratory scale can actually be regarded as batch processes. This makes the scale-up calculations more straightforward. The presented framework focuses on reactions under heating or room temperature only and the most important in- and outputs from an LCA perspective to such a heated liquid batch reaction process are illustrated in Fig. 2.

An entire reaction process normally consists of multiple process steps. The reaction step itself, where the target product is formed, is followed by processing, purification and/or isolation steps to obtain the required product. It is the reaction step, which takes place in the batch reactor. Material inputs are reactants, solvents and possibly catalysts whereas the energy input is mainly required for heating

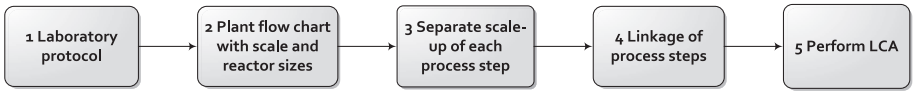


Fig. 1. Overview of scale-up procedure.

Table 1
Translation of laboratory to large-scale processes according to the presented framework.

Laboratory scale process	Scaled-up process according to framework
Reaction under heating	Heated liquid batch reaction in an insulated batch reactor with an in-tank stirrer
Mixing (magnetic stirrer) Dispersing	In-tank stirring
Blending Mixing (viscous solution) Homogenizing (all types) Dispersing	Rotor-stator type homogenizer
Pestling in mortar Grinding/milling Other particle size reduction	Grinding
Filtration (e.g. membrane, reverse osmosis, dialysis) Sieving Centrifugation/cyclonic separation Other solid–liquid separation	Filtration/centrifugation
Distillation (Rotary evaporation)	Distillation
Vacuum drying Drying Rotary evaporation	(Oven) drying/vaporization
(Manual) Transferring of liquids	Pumping
Waste disposal	Pre-treatment (case specific) Solvent recycling – distillation Solvent recycling – filtration Co- and by-product isolation
Normally not included in laboratory process	Heat recovery through heat exchangers

and stirring of the reaction mixture. The main output of this reaction is a reaction mixture containing all the products (target product and eventual co-/by-products) according to the reaction equation, solvent, unreacted educts (reactants), catalysts and, in certain cases, other products from side reactions. Other outputs of the reaction are waste heat and emissions to air.

While the reaction itself is already completed during the reaction step, the target product still needs to be isolated from the reaction mixture. This usually requires processing, isolation and/or purification steps, which in turn may use additional energy and material inputs. Besides the target product, the output of those steps might comprise by- and co-products, waste heat, wastewater, other waste (including hazardous waste) and emissions. Some of the material and heat waste can be recovered and reused as inputs within the same process step (intra-step-recycling) or within the reaction process (inter-step-recycling).

A chemical production plant is rarely based on a single reaction process but it consists of multiple reaction processes. This means that the product of one process serves as an input for the next reaction process (Fig. 3). Heat and material recovery can also be

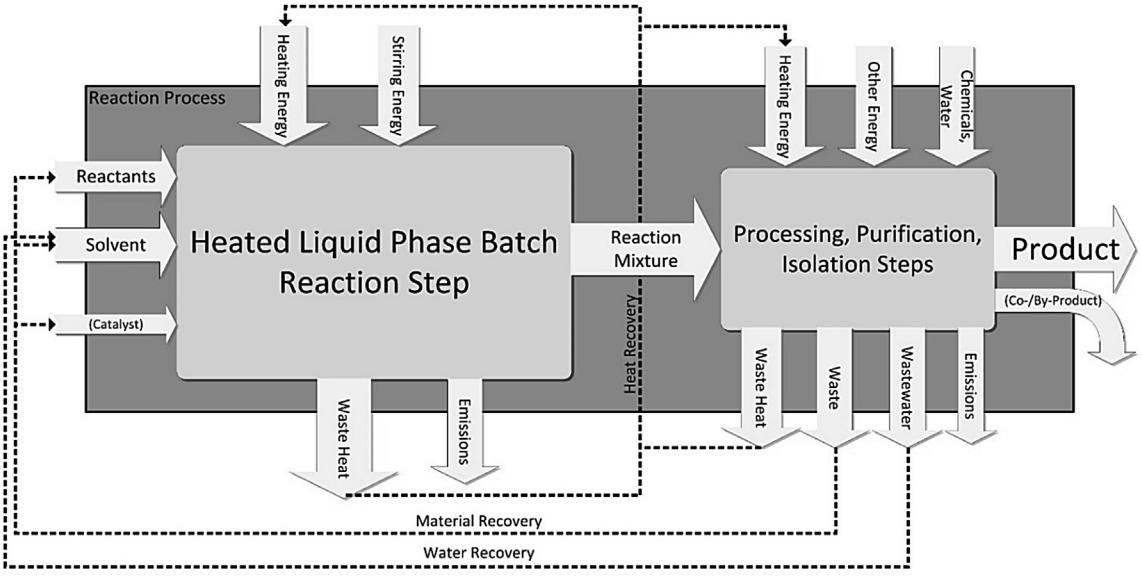


Fig. 2. Material and energy in- and output of a heated liquid phase batch reaction process.

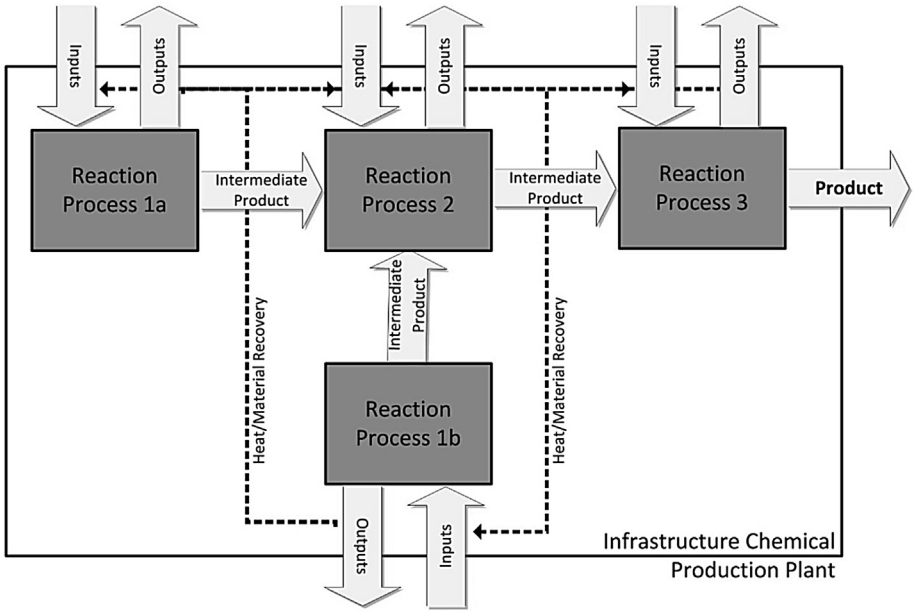


Fig. 3. Schematic structure of a chemical production plant with multiple reaction processes.

performed across different reaction processes (inter-process-recycling). As a last input to the LCA, the contribution of the infrastructure of the entire plant must be included in the consideration.

2.1. Input values – reaction step

2.1.1. Reactants

The scale-up of each reactant is performed linearly because those have to be used in stoichiometric quantities according to the lab procedures. Even in cases where the laboratory procedure uses one reactant in excess (more than the stoichiometric amount), a linear scale-up is applied. The excess use of one reactant is normally used in order to assure that the conversion takes (fully) place. Therefore, it is important to use the same relative amount in the larger scale. For the production of the reactants themselves, datasets for several commonly used chemicals should be used where available. If no data for a certain chemical is available, generic average datasets (e.g. for organic or inorganic chemicals) can be used instead in a first phase (Hischier et al., 2005). Another possibility is to model the production of such a chemical also according to the here described framework. This latter approach is especially beneficial if the chemical is expected to deviate considerably from the average data and is used in significant amounts that is expected to have a relevant impact to the end results.

2.1.2. Solvents

A solvent is needed for every liquid batch reaction. In contrast to the reactants, solvents – unless they are being used simultaneously as one of the reactants – are not used in stoichiometric amounts. Since small quantities are normally processed at the lab scale, the relative amount of solvent used there is higher than on the industrial scale. To incorporate a more efficient use of solvents, this framework uses a 20% relative solvent reduction for the scale-up, unless an exact concentration is needed in which case the solvent has to be scaled linearly. This number is an estimate based on expert opinion and can be used when there is no further knowledge about the amounts of solvents used at the industrial scale. However, in the event that more accurate data are available, it is preferable to use such information.

In many cases, solvents can be regained after the reaction through distillation or a filtration, but such a solvent recycling is rarely a part of the lab process. Closed circles for inter- or intra-process-step recycling can thus be modeled for the scale-up. This reduces the solvent input further – besides the scaling dependent reduction – by the amount of the recycling rate. However, the energy for the regaining process, whether its distillation or filtration, has to be included. This is described more accurately in the appropriate section (e.g. see *Distillation* below). Other possible handling of the contaminated solvents as hazardous waste is described in the according LCA output section. Where high solvent purity is needed, the solvent might not be reused in that same process due to contamination.

2.1.3. Catalysts

Catalysts are crucial for the success of several reactions. At the same time, they are mostly used in very small amounts and in many cases not affected by the reaction. Catalysts often contain transition metals, for example platinum, with a significant environmental impact and high purchase prices. The efforts to regain the catalyst in the laboratory scale would in several cases not be justified because of the very small amounts used. Therefore, the laboratory procedure rarely deals with the problem of recycling. This situation might change in an industrial scale where catalysts are applied in kg amounts. Suddenly, recycling of catalysts becomes a concern. Therefore, in a scale-up it has to be assessed whether a catalyst could be recycled with minor efforts and an according procedure needs to be modeled where reasonable. This information can be obtained from the researchers directly if available. When no such information can be obtained, one should assume as a first step that the catalyst is not recycled and evaluate how it affects the end-results of the LCA through scenario analysis.

2.1.4. Heating energy

The total amount of energy needed depends on many factors. It can vary significantly depending on the reactor (type, size, surface, material, insulation), the heating element (type, size, surface, material, efficiency), or the reaction parameters (amount, temperature, time, specific heat capacity of reaction mixture, endothermic/

exothermic). Many of these factors (e.g. reactor, heating element) depend more on the actual plant design than on the reaction itself. Hence, an exact calculation of their values is only possible if a detailed plant design is available. For the scale-up framework, we handled this whole complexity by simplifications, focusing on the main contributors and working with average designs and sizes. This opens the possibility to estimate those scaled-up values, which are necessary for the LCA, without a detailed plant design.

The heating energy required is composed of the energy to raise the reaction mixture to a certain temperature and to keep it for the duration of the reaction (Q_{react}). This is calculated as the sum of the energy for raising the temperature (Q_{heat}) and the heat loss on the reactor surface (Q_{loss}) divided by the efficiency of the heating device (η_{heat}) (Equation (1)). Here, the efficiency of the heating device is the ratio between the energy actually transferred to the reaction mixture and the amount of energy that is consumed by the heating element, taking into account an eventual heat recovery from direct exhaust gases.

$$Q_{react} = \frac{Q_{heat} + Q_{loss}}{\eta_{heat}} \quad (1)$$

2.1.4.1. Energy to reach the reaction temperature Q_{heat}. The specific heat capacity of the main solvent is used as a basis for the calculations given the examined reaction takes place in a solution. If the solvent consist of a mixture, the specific heat capacity of that solvent mixture can be estimated as mole fraction average of the pure components (although this neglects the excess heat capacity) (Green and Perry, 1934). Reducing the heat capacity to that of the main solvent only is a simplification used for the purpose of the framework and neglects the influence of other/the reactants as well as minor solvents. The specific heat capacity (C_p [J/kg·K]) indicates the amount of energy that is required to obtain a temperature change of 1 K per unit mass (kg) of material. With the reaction temperature (T_r), the starting temperature (T_0; usually ambient temperature at 25 °C = 298.15 K if the feed is not coming from a previous step with a different temperature) the mass of the reaction mixture (m_{mix}) and the specific heat capacity of the solvent, the heat can be calculated according to Equation (2).

$$Q_{heat} = C_p{*}m_{mix}{*}(T_r - T_0) \quad (2)$$

Normally, the reactor is not filled completely, leaving a certain amount of air (or depending on the reaction e.g. nitrogen gas) which will be heated as well. However, the mass of this gas is extremely low compared to the reaction mixture in a filled reactor, leading to a low contribution that can be neglected in the procedure here.

2.1.4.2. Energy to compensate the heat loss Q_{loss}. Heat is lost through the surface of the reactor and must be compensated by additional heating in order to keep the temperature at the same level. For our model, we assume a model in which a reactor is insulated over its entire surface. A reactor made, for example, of stainless steel is insulated with an outer layer of insulation material. The heat that is lost has to pass through the reactor wall and the insulation to reach the ambient air outside the reactor. Depending on the heating system – e.g. a heating coil inside the reactor or a jacket around it – the heat loss varies. As a simplification, we neglect the conduction through the reactor walls and only consider the insulation, it being the limiting factor. To calculate the heat loss (Equation (3)), the surface area of the reactor (A), the thermal conductivity of the insulation material (k_a), the thickness of the insulation (s), the temperature difference between the inside and outside of the reactor ($\Delta T = T_r - T_{out}$) and the time of the reaction (t) are needed.

$$Q_{loss} = A{*}\frac{k_a}{s}{*}(T_r - T_{out}){*}t \quad (3)$$

Together with Equation (1), Equations (2) and (3) can be put together to form Equation (4):

$$Q_{react} = \frac{Q_{heat} + Q_{loss}}{\eta_{heat}} = \frac{C_p{*}m_{mix}{*}(T_r - T_0) + A{*}\frac{k_a}{s}{*}(T_r - T_{out}){*}t}{\eta_{heat}} \quad (4)$$

However, in most of the cases where a lab production is analyzed, large parts of the above-mentioned information is not known in detail. To nevertheless be able to calculate such scaled up reaction data, Table 2 lists average data that can be used as a best approximation based on the required scale.

While all the parameters to calculate Q_{heat} are solely reaction specific data (and therefore have to be adapted for every single reaction), Q_{loss} is additionally influenced by the reactor size and design. Assuming a cylindrical reactor, the surface area (A) can be calculated with the diameter (D) and height (L). The minimal surface at a given volume is obtained at a ratio between the diameter and height of one, which was used as the calculation basis.

The actual volume of a reactor ($V_{(reactor)}$) normally exceeds the quantity that is processed in there ($V_{(mix)}$). By default, a 10% higher reactor volume compared to the reaction mixture volume was applied based on expert estimates.

Different insulation materials exist that can be used with varying thicknesses. The material is usually chosen depending on the temperature whereas the thickness is decided by the economic thickness of insulation – which calculates the costs of the material in comparison to the costs of energy loss and determines the appropriate size – as well as the critical thickness – below which the heat loss with insulation is greater than without due to the increased surface. Fiber glass is a widely used insulator in the industry with a temperature range of 20–450 °C and thermal conductivity between 0.032 and 0.052 W/(m × K) (Thirumaleshwar, 2009). All the reactors in Table 2 are calculated using a glass fiber insulation of 75 mm thickness (Perry and Green, 2008).

The heating element's efficiency depends on several factors, such as type, material, fluid and temperature. We standardized this value at 75% for the 1′000 l reactor and scaled it with a scaling factor of 0.02 that was found for log furnaces, being the best approximation for which a scaling factor was available (Caduff et al., 2014).

With the amount of data available, the calculation of Q_{react} for a certain scale becomes a simple procedure. Remaining parameters that must be identified individually for each reaction are the specific heat capacity (C_p), the mass of the reaction mixture (m_{mix}), the reaction temperature (T_r) and its time (t). For example, to obtain the overall heat to perform a reaction at a certain temperature in a 1′000 l reactor, Equation (4) can further be specified by Equation (5)

$$Q_{react(1000\ l)} = \frac{C_p{*}m_{mix}{*}(T_r - 298.15\ \mathrm{K}) + 3.303\ \mathrm{W/K}{*}(T_r - 298.15\ \mathrm{K}){*}t}{0.75} \quad (5)$$

Table 2
Suggested scale-dependent data for the calculation of heating energy.

Physical entity	Symbol	Unit	100 l	500 l	1′000 l	5′000 l	10′000 l
Reaction mixture volume	$V_{(mix)}$	m^3	0.1	0.5	1	5	10
Height of reactor	L	m	0.519	0.888	1.119	1.913	2.410
Diameter of reactor	D	m	0.519	0.888	1.119	1.913	2.410
Surface area	A	m^2	1.271	3.716	5.899	17.249	27.381
Reactor volume	$V_{(reactor)}$	m^3	0.11	0.55	1.1	5.5	11
Insulation material	–	–	Glass fiber	Glass fiber	Glass fiber	Glass fiber	Glass fiber
Thermal conductivity of insulation	k_a	$\frac{W}{m*K}$	0.042	0.042	0.042	0.042	0.042
Insulation thickness	s	m	0.075	0.075	0.075	0.075	0.075
Heat transfer coefficient of insulation	k_a/s	$\frac{W}{m^2*K}$	0.56	0.56	0.56	0.56	0.56
Efficiency of heating element	η_{heat}	%	72%	74%	75%	77%	79%
Impeller diameter	d	m	0.173	0.296	0.373	0.638	0.803
Rate of heat loss per Kelvin	$\frac{A*k_a}{s}$	$\frac{W}{K}$	0.712	2.081	3.303	9.659	15.333
Starting and outside temperature	$T_0 = T_{out}$	K	298.15	298.15	298.15	298.15	298.15

Depending on the process, the secondary energy source (gas, oil, fuel, electricity etc.) used to provide the calculated energy is chosen. If there is no knowledge about the appropriate energy source, natural gas should be selected as it is used in over 75% of all the process heating in manufacturing within the US (Energy Information Administration, 2006).

2.1.5. Stirring energy

During a reaction, a certain amount of stirring energy is consumed. Factors influencing the stirring energy are type (N_p) and diameter (d) of the impeller, the rotational velocity of stirring (N), the density of the reaction mixture (ρ_{mix}) as well as the reaction time (t). Since some energy loss occurs, for example through friction, from the electricity input to the actual stirring, an efficiency value (η_{stir}) is included. Their mathematical relation is shown in Equation (6), resulting in Joules when applied with SI-units (Zlokarnik, 2000).

$$E_{stir}[J] = \frac{N_P * \rho_{mix} * N^3 * d^5 * t}{\eta_{stir}} \quad (6)$$

The power number N_p is a dimensionless number according to the theory of dimensional analysis. It is specific to a certain type of impeller and constant at turbulent flow. Turbulent flow is commonly used in mixing, unless a highly viscous material is being processed. For this framework, only stirring at turbulent flow is considered, leaving the power number constant for the calculations.

Based on the data used above, the density of the reaction mixture is calculated as the ratio of the mass of the reaction mixture (m_{mix}) and its volume ($V_{(mix)}$).

An axial flow impeller, such as a hydrofoil type, is used as an average stirrer type (Table 3). The corresponding power number has been found to be in the range between 0.28 and 1.94 of which the average was calculated (Albright, 2009). The power number for a radial flow is higher.

The impeller diameter was calculated based on the assumption that it measures one third of the reactor diameter. A rotational speed of 85 rpm for the 1′000 l reactor is assumed and this entity was calculated for the other scales based on equal tip speed (i.e. assuming $\pi * d^2 * N = constant$).

Applying the data to a 1′000 l reactor with an axial flow impeller, Equation (6) is thus transformed into Equation (7).

$$E_{stir(1000\ l)} = \frac{0.79 * \rho_{mix} * 1.417^3\ s^{-3} * 0.373^5\ m^5 * t}{0.9} = 0.0180\ m^5 s^{-3} * \rho_{mix} * t \quad (7)$$

2.2. Input values – processing, purification and isolation steps

Once the reaction has occurred, the production of the chemical is not terminated. Usually, there are subsequent isolation and purification steps needed in order to obtain the final product. Even before the reaction takes place, some processing and preparation of the reagents might be needed. To account for such subsequent steps, we present in the following sections estimation values based on different calculations and considerations.

2.2.1. Homogenizing

Different types of homogenizers, such as the high pressure, the ultrasonic and the rotor-stator type homogenizer, can be distinguished. In this framework, only the rotor-stator type is included. This type can be regarded as stirring at very high shear rates. The calculation of the energy requirement for homogenizing, therefore, utilizes the same equation (Eq. (6)) as in the case of stirring. Only the parameters have to be adapted whereas the standardized values listed in Table 4 can be used. The power number data is comparable to normal agitators and an average power number was calculated (Myers et al., 2001; Zhang et al., 2012). However, in comparison to conventional agitators, the impeller diameters of a

Table 3
Suggested scale-dependent data for the calculation of the stirring energy.

Physical entity	Symbol	Unit	100 l	500 l	1′000 l	5′000 l	10′000 l
Impeller diameter	d	m	0.173	0.296	0.373	0.638	0.803
Power number of impeller	N_p	–	0.79 Axial flow	0.79 Axial flow	0.79 Axial flow	0.79 Axial flow	0.79 Axial flow
	N_p	–	3.44 Radial flow	3.44 Radial flow	3.44 Radial flow	3.44 Radial flow	3.44 Radial flow
Rotational speed of agitator	N	1/s	3.052	1.785	1.417	0.828	0.658
Efficiency of agitator	η_{stir}	%	90	90	90	90	90

Table 4
Suggested scale-dependent data for the calculation of the rotor-stator homogenizer energy draw.

Physical entity	Symbol	Unit	100 l	500 l	1′000 l	5′000 l	10′000 l
Impeller diameter	d	m	0.072	0.111	0.139	0.260	0.288
Power number of rotor	N_p	–	2.39	2.39	2.39	2.39	2.39
Rotational speed of rotor	N	1/s	48.333	48.333	48.333	20	20
Efficiency of agitator	η_{stir}	%	90	90	90	90	90

homogenizer are smaller. We consulted producer data to determine an average value for the diameters and shear rates, assuming 0.9 rotor-stator ratio (based on maximum value that was encountered), where the impeller information was not available, and at maximum shear rate. The increased shear rate, in comparison to stirring, results in a considerably higher energy consumption. Given this much higher energy consumption, homogenizing steps can have a considerable influence on the LCA's overall result. As the impeller diameter is raised to the fifth power for the energy use calculation, already a small change alters the value considerably. Therefore, a sensitivity analysis is advisable, which can be complemented with the results of producer data for homogenizers.

2.2.2. Grinding

Energy consumption mainly depends on the size of the final particles, the material to be grinded and the type of grinding. We calculated an average value of various grinders (Vauck and Müller, 2000), resulting in a value of 8–16 kW h/ton of grinded material. Lacking any information about the particles, the upper value (i.e. 16 kWh/ton) should be used as a conservative approximation and complemented with scenario analyses.

2.2.3. Filtration and centrifugation

The inputs are energy and a certain amount of liquid to wash the filter cake. Depending on the need and preferences of a specific production plant, different types of filters are available on the market. Various factors have an influence on the energy consumption, the main contributor being the particle size. Smaller particles use more energy, while larger grain filtrations require less. Fine particle and paste-like material are the most energy intensive. Alt (2000) estimates the energy consumption of filters, including all equipment, in the range between 1 and 10 kWh per ton of dry material. Centrifugation is a solid–liquid separation procedure, similar to a filtration. With the same conditions as in a filtration, the energy consumption of a centrifuge is expected to be slightly higher. During the experimental laboratory procedure, a researcher normally builds an understanding whether the filtration is energy intensive or not, facilitating the estimations. However, if this information is not available, the upper value (10 kWh/ton) should be used. Since the presented energy requirement can differ by a factor of ten, it is appropriate to make sensitivity analyses including the average value (5.5 kWh/ton) and, possibly, also the lowest case in order to understand what the contribution of the filtration to the impact of the whole plant is.

2.2.4. Distillation

Distillation involves heating of the compound to the boiling point of the targeted material with subsequent cooling for the condensation in order to recover the liquid. The heating energy can be obtained using an analogous calculation as in the case of the reactor heating. The main difference is that additional heat (Q_{vap}) is required for the enthalpy of vaporization (ΔH_{vap} [J/kg]) that is needed to convert the material from the liquid to the gaseous state. Furthermore, a certain amount, known as the reflux, of the vaporized solvents is condensed and fed again into the distillation column.

Whereas for the calculation of Q_{heat} the mass of the whole mixture or feed compound is needed, Q_{vap} only comprises the mass of the liquid (m_{dist}) that needs to be vaporized, i.e. the distillate (Equation (8)).

$$Q_{vap} = \Delta H_{vap} * m_{dist} \tag{8}$$

The reflux ratio (R) is known as the ratio between the liquid reflux flow (L) divided by the distillate (D) and is dependent on the composition of the waste solvents, the required purity of the distillate and the difference between the boiling points of the various solvents. For each distillation of a binary system, a minimum reflux ratio (R_{min}) can be calculated with the Underwood equation, which indicates the lowest ratio for which the distillation can take place (Equation (9)) (Underwood, 1949). In the case of a multicomponent distillation, the calculation becomes more complex. For the sake of simplicity of this scale-up framework, such distillations should be treated as sets of binary systems, resulting in a separate reflux ratio for each set. Since the actual reflux ratio is very case specific and can vary considerably, it is difficult to obtain an average value. The closer the actual reflux ratio comes to the minimum, the lower the energy consumption. However, from an economic perspective, a ratio between 1.1 and 1.3 times as high as R_{min} seems to be to most feasible and is commonly used (Capello et al., 2005), which is why a value of 1.2 is used for the here described framework.

$$R_{\min} = \frac{1}{\alpha - 1}\left(\frac{X_{LD}}{X_{LF}} - \frac{\alpha * (1 - X_{LD})}{1 - X_{LF}}\right) \tag{9}$$

α: relative volatility of the solvents (>1); x_{LD}: target purity of distillate (molar fraction); x_{LF}: molar fraction of target compound in feed.

In the calculation of the heating energy for the distillation (Eq. (10)), the reflux ratio means that the enthalpy of vaporization has to be overcome more than once, according to the determined ratio. In contrast to the reaction time (t), the duration of the distillation is difficult to predict given that the setup, material, size, surface, reflux ratio etc. play an important role. For the sake of the scale-up framework, Q_{loss} is excluded from the equation. Nonetheless, the heat loss has to be considered. A 10% lower efficiency (expert estimate) of the heating element (Eq. (10)) is chosen to reflect the heat loss. To use a less complex setup, a distillation in an industrial plant is preferably performed at ambient pressure rather than using a vacuum or pressurize. This is possible as long as the boiling temperature of the required liquid does not exceed a certain value (approximately < 200 °C) and the differences between the boiling temperatures of the materials to separate are clearly distinct.

$$Q_{dist} = \frac{Q_{heat} + Q_{vap} * (R + 1)}{\eta_{heat} - 0.1} = \frac{C_p * m_{mix} * (T_{boil} - T_0) + \Delta H_{vap} * m_{dist} * (1.2 * R_{\min} + 1)}{\eta_{heat} - 0.1} \tag{10}$$

An empirical study of waste solvent distillations in Switzerland

showed that on average 1.53 kg of steam are required for each kg of waste solvent in a batch distillation (Capello et al., 2005). However, these values range from 0.81 to 2.81 kg of steam, which indicates that the consumption is very case specific. In the case where the heating energy cannot be calculated with the aforementioned equations due to lack of information, this empirical value (1.53 kg steam/kg waste solvent) can be used for the scale-up. For the conformity of this scale-up framework and to obtain case specific values, it is advisable to calculate the distillation energy with the presented equations whenever possible. Comparison of the calculations with the empirical data can then be used for scenario analyses.

To consider the condensation of the liquid, cooling water with an average of 0.027 kg per kg of waste solvent can be used as an input to the LCA, which has been determined empirically (Capello et al., 2005).

2.2.5. Drying

Drying of solids requires the vaporization of the remaining wet fraction that has not been removed in the previous steps (e.g. filtration). Depending on the setup, the type of dryer and heat recovery, there is a considerable variation between the efficiency of a drier ranging from as low as 30% to even exceed 100% (with efficient heat recovery) (Grant, 2000). Similar to the case of the distillation, energy is required to raise the temperature of the liquid to the boiling temperature plus its enthalpy of evaporation (Eq. (11)). Given the definition of the drier efficiency (η_{dry}) (i.e. the ratio between the heat required to vaporize the removed liquid and the heat used), only the heat required to raise the temperature of the liquid is considered. Hence, the heat loss is already comprised in the efficiency, for which a value of 80% was chosen as a standard value (expert estimate). The mass of the solvent to be evaporated is obtained by comparison of the weight before the drying step with the weight afterwards as stated in the lab protocol. In certain cases, for example when the solid material is heat sensitive, a vacuum might be required to lower the boiling temperature. This results in less heating energy required. However, this effect is counterbalanced by the energy used for the vacuum pump.

$$Q_{dry} = \frac{C_{p,liq} * m_{liq} * (T_{boil} - T_0) + \Delta H_{vap} * m_{vap}}{\eta_{dry}} \tag{11}$$

2.2.6. Transfer of liquids (pumping)

The reaction mixture, liquids, reagents etc. used in the reaction often have to be transported between process steps. If it is a liquid or a gas phase, this transfer normally occurs in pipes whereas the energy comes from a pump. The change in the hydraulic head (Δh) dictates the energy consumption of a pump. It is composed of the difference in the gravitational head (Δh_g) – the height difference between A and B –, the dynamic head (Δh_{dyn}) – influenced by the average speed of the fluid (v) –, the static head (Δh_{st}) – formed by the pressure differences of A and B – and the frictional head (Δh_{fr}) – pressure loss through friction depending on the friction factor (λ), pipe length (l) and diameter (d) as well as the average speed (v). Equation (12) shows the calculation of the change in the hydraulic head. The friction factor varies between laminar ($Re < 2320$ with $Re = \frac{v*d}{v_{liq}}$; v_{liq}: kinematic viscosity of fluid) and turbulent flow and the material of the pipe (k; surface roughness) (Vauck and Müller, 2000). With the efficiency of the pump (η_{pump}), consisting of the hydraulic, volumetric and mechanical efficiency, the mass to be transferred (m) and the gravitational acceleration (g) the energy consumption in turbulent flow is obtained following Equation (13).

$$\begin{aligned}\Delta h &= \Delta h_g + \Delta h_{dy} + \Delta h_{st} + h_{fr} \\ &= \Delta h_g + \frac{(v - v_0)^2}{2*g} + \frac{\Delta p_{st}}{\rho * g} + \lambda * \frac{l}{d} * \frac{v^2}{2*g}\end{aligned} \tag{12}$$

$$E_{pump} = \frac{m*g*\Delta h}{\eta_{pump}} \tag{13}$$

The parameters of the pipe have been standardized for the framework to a diameter of 0.2 m, a length of 30 m and steel as material ($k = 0.1$ mm) (Vauck and Müller, 2000). The height difference for the gravitational head (Δh_g) was standardized to 4 m, thus ensuring that the height of all the above-proposed reactor sizes can be overcome. Using an average speed of 1 m/s at turbulent flow, the hydraulic head results in 4.2 m. This value for the hydraulic head is used as the standard calculation basis to estimate the energy consumption of a pump, with an efficiency of a reciprocating pump lying between 0.7 and 0.85 (Vauck and Müller, 2000). By these means, 55 J are required per kg of pumped material (Eq. (14)).

$$E_{pump} = \frac{m*9.81\ \mathrm{m/s^2}*4.2\ \mathrm{m}}{0.75} = 55\frac{\mathrm{J}}{\mathrm{kg}}*m \tag{14}$$

2.2.7. Other processes

The framework only covers a certain amount of processes in its scale-up. Therefore, those processes that are excluded here – for example ion exchange, ultra-sonication, wet spinning, degassing and others – should be scaled, as a best approximation, using the data from known similar processes or data from machinery that could potentially be used to perform the task. This kind of data can be obtained from producers of the corresponding machinery.

2.3. Output values

2.3.1. Reaction mixture

The reaction mixture describes the output of any process step (e.g. the reaction step) containing the target compound of a reaction process, which is not in an isolated form. The reaction mixture is used as an input for subsequent processing, isolation and/or purification steps, which ultimately isolate the target compound. It might contain excess heat after the heated reaction if it is not needed for the subsequent steps and can therefore be used for the heat recovery (see below).

2.3.2. Product/yield

The product does not necessarily have to be a final product. It can be an intermediate product serving as a starting material for another reaction process (Fig. 3). Generally, one could assume that from the laboratory scale to an industrial production plant, the fractional yield of the desired product should increase given that lab experiments exploring new materials normally focus on the proof of concept rather than the optimization of the production yield. However, this conclusion is not that trivial. An industrial production might aim for high purity of the end product, which could involve additional purification steps, resulting in an even lower yield compared to the lab experiments. The degree by which the yield changes from a laboratory scale to an industrial production depends on several factors. Those factors comprise, among others, the required purity, price/value of the material, type and number of involved steps or the type of reaction. Defining a universally applicable prediction about the yield behavior in chemical processes is therefore difficult. The specific process examined has

to be taken in consideration and estimated accordingly based on a stepwise procedure. This in turn requires a deep understanding of the process itself. For the purpose of this framework, we suggest to compare the yield to a similar and existing large-scale process, helping with the prediction of the yield. Similar in this context is meant from a chemical or technical perspective, e.g. to predict the yield of a new polymerization reaction, an existing polymerization reaction process could be used as an approximation. Either the process as a whole is compared or single process steps alone, which are then compiled. In the event that this kind of information is not available, the best existing information should be used, meaning the same yield as in the lab protocol.

2.3.3. Co- and by-products

It is quite common in chemical reactions that apart the wanted product, one or several further products can result from the overall reaction. Such further products can potentially be used as inputs for other process systems. In such a case, one must decide how to handle this topic within the LCA. Depending on its economic value, such further products are seen either as co-products (i.e. having a similar economic value as the wanted product) or a by-product (i.e. having a clearly lower economic value). Options in case of a co-product are either allocation or system expansion. For a by-product, it is possible to model it as a flow that leaves the examined system and is therefore outside of the system boundaries. This means that it is cut off without further environmental burdens or credits. Hence, the LCA practitioner performing the scale-up has to decide which of the two perceptions is the more appropriate one for the specific case. Ultimately, a context specific reasoning based on the scope and goal of the study, the quality of information and data, the amount and importance of the co-/by-product etc., should be applied. In those cases, scenario analyses are a useful and important tool to understand the impact of the modeling decision.

If there is no reason to expect it differently, the same co- and by-products should be assumed and scaled linearly according to the target product.

2.3.4. Waste and recovery

Waste (especially hazardous) is expected in several chemical processes. There are different scenarios that can occur with such waste at a chemical production plant. A waste consisting of a considerable amount of solvent, could be (partially) regained and re-used through distillation. Although this depends on the specific setup, the waste composition and the solvents, a recovery rate of 68% can be expected on average based on empirical values (Capello et al., 2005). With this recovery rate, the solvent input can be reduced by the same amount. In many cases, however, a considerably higher recovery rate can be expected and a more case specific estimate should be used where reasonable. To improve the robustness of the results, we suggested to search for information about the possible recycling rate of the specific solvent under consideration. When including a distillation scenario, the energy consumption – described in the distillation section above – needs to be accounted for in the LCA.

Incineration of the solvent waste at the production site itself is another option. The obtained heat can be utilized, for example to pre-heat processes. With the solvent's enthalpy of combustion, the generated heat can be calculated and included as a negative energy input to the LCA. Additionally, a certain amount of slag might result as waste from the combustion.

A third option is to treat it as hazardous waste. In the LCA, this includes modeling it to end-up in a hazardous waste incineration plant. As a conservative approach in this framework, all the waste that does not contain (or not a lot of) solvent should be modeled to a hazardous waste incineration plant, unless it is clear that it is not contaminated. Only if it is clear that the waste is not contaminated, can it be treated as “regular” waste.

The treatment of solvent waste in a production plant usually is motivated by economic reasoning first. An on-site solvent recycling process, e.g. via distillation, involves further distillation columns which in turn require an investment and must be operated. Those additional processes and machineries bear an enhanced risk for accidents. At the same time, the energy costs for the distillation itself must be advantageous compared to the purchase of new solvent and disposal of the waste. Anticipating which option is the most appropriate is therefore difficult although it has been shown that solvent recovery can result in a positive environmental impact (Raymond et al., 2010). Also in this case, a scenario analysis, for example one scenario being all the solvent waste to a hazardous waste incineration plant and the other including a recovery, can be very helpful and should be included to improve the results of the study.

2.3.5. Wastewater

Many chemical production plants have an on-site system to collect and pretreat wastewater before it is released as wastewater (into a treatment plant) or reused. Several different treatments exist depending on the type and quantity of contamination. Including a detailed plan for the on-site wastewater treatment would go beyond the scope of this paper. Obviously, if data of similar processes exist, it can be used to simulate the on-site wastewater treatment process.

As a simplification, the following options have been elaborated for wastewater treatment within the LCA study. Processes performed in aqueous solution without contamination with hazardous substances can be modeled to end-up in a wastewater treatment plant. However, contaminated wastewater should be treated as hazardous waste.

The wastewater quantity can be reduced through a recycling process. At the same time, the water input for the process is reduced by the recycling rate, analogously to other solvents recycled. Depending on the purity of the water needed and its contamination, a filtration might be adequate as a recycling procedure. Another option is to recover the water through distillation. The wastewater treatment plant option is preferable when lacking the appropriate information.

2.3.6. Air emissions

Direct emissions of chemical substances from the process into air, water or land can have a major environmental impact if not treated properly. Emissions are highly process and reaction specific. To identify possible emission sources, every step in the process should be challenged accordingly. Especially, the steps involving combustion since gases might be emitted. Further air emissions can occur from by-products of chemical reactions (e.g. gas building), volatile (organic) solvents, decomposition and unreacted parts. Whereas the by-products are easily detectable in the reaction equation, the other group are not as easily recognizable and/or quantifiable. When identified, the design of a plant should include, where appropriate, a trapping of the compound (e.g. gas) to reduce the emission potential. In the laboratory, this is usually neglected, making it more difficult to identify those sources from the lab protocol.

Fugitive emissions comprise unanticipated releases of chemicals deriving from different sorts of leaks. Various methods to estimate fugitive emissions exist. The US Environmental Protection Agency (US EPA) identified process operations, storage tanks, equipment leaks, wastewater collection and treatment, cleaning, solvent recovery and spills as possible air emission sources and suggested a method to estimate those quantities (EIIP, 2007). Shine (1996)

proposes methods to estimate air emissions of volatile organic compounds in batch processes. Hassim and co-workers (2010 and 2012) proposed a method to estimate the fugitive air emissions based on the level of detail of the plant design. Although the latter method focuses on continuous processes, certain estimates and procedures can be adopted in this scale-up. For this stage, the procedure for the simple plant flow diagram may be used. This procedure includes pre-calculated fugitive air emissions for standard process modules and assumes that the stream consists of 100% of its worst chemical. Sensitivity analyses using an emission reduction technique and comparing it to the production without it, gives an indication of the impact and importance for the specific case.

2.3.7. Waste heat

Heat recovery is a broadly used technique in chemical production plants to improve the energy efficiency. Every process step involving heating has a potential for heat recovery. During the plant flow chart compiling step within this framework, it is advisable to consider possible recovery routes for heat using heat exchangers. The heat is obtained from heated process and waste streams or the heating itself, e.g. through combustion gases. The heat recovery of the latter is already part of the heating element's efficiency within this framework. Therefore, heat recovery from process and waste streams is only considered during this step. The energy is obtained as heat, reducing the heating energy requirement of the same or another process step by the same amount for the LCA input.

Pinch analysis is a common technique used in the industry to significantly reduce the energy requirement of a production plant (Ebrahim and Kawari, 2000). At the point of such an LCA scale-up, the production plant does not exist and is not planned, preventing a detailed pinch analysis. Nevertheless, with advanced knowledge in pinch analysis, it is still possible to perform one in a simplified manner, allowing for the detection of heat recovery opportunities.

However, for this framework we suggest a simpler approach without the need of detailed knowledge of pinch analysis. Only heat that is contained in excess in the reaction mixture, being the output (e.g. a reaction at 90 °C) of the reaction step, compared to the required temperature of the subsequent processing step (e.g. filtration at room temperature) is considered here. It is not the goal of this framework to obtain an LCA for the most energy efficient production process possible but the simulation of the production from an LCA perspective at a larger scale. A conservative approach (use rather lower recovery rates) is therefore advisable when including a heat recovery scenario. This assures that the results are rather overestimated resulting in a higher environmental impact. The most conservative approach, however, would be not to include heat recovery at all. Also in this case, a scenario analysis can be helpful in understanding the impact of the decisions.

2.4. Infrastructure

Including the impact associated with the construction of the plant equipment and its infrastructure, completes the LCA of such a production plant. Lacking knowledge of the actual production plant means that a generic dataset for a chemical plant should be used. One such dataset – offered by *ecoinvent* – consists of the average from two different chemical plants (Weidema et al., 2013). One unit of said dataset stands for a production plant with a lifetime of 50 years and an average annual output of 50′000 tons, resulting in an output of 2.5 million tons over the whole lifespan. Linear scaling of this input value based on the simulated production plant's annual output should be used to account for the size. However, it has to be borne in mind that the suggested infrastructure input data is not case specific as two chemical plants with the same annual output but with different products and processes might differ considerably in size.

2.5. Summary

Using the described calculations and estimates, summarized in Table 5, help to facilitate a scaled up LCA study of a laboratory chemical production. It is important to stress that the heat and waste recovery simulations should be included at the end after all in- and outputs have been compiled.

3. Scale-up example

In order to illustrate the application of the framework, we use a simple fictional example and analyze the scale-dependency of the results. The catalytic reaction between compound A and B follows Equation (15):

$$A + 2B \xrightarrow[\text{Catalyst}]{\substack{H_2O \\ 60^\circ C}} 2C \qquad (15)$$

In the laboratory, 870 mg (5 mmol) of reactant A are added to 660 mg (10 mmol) of reactant B. 1.9 mg (0.005 mmol, 0.001 equivalents) of catalyst are dissolved in 250 ml of H_2O and the solution is added to the reactants. The reaction mixture is stirred for 2 h at 60 °C. After cooling down to room temperature, the reaction mixture is filtered and a wet filtercake of 1.503 g is obtained. Further drying results in 1.423 g (9.3 mmol, 93%) of the target compound C.

3.1. Scale-up using the framework

To scale this process to a processing quantity of 100 l, a simple plant flow chart has to be designed (Fig. 4). The reaction takes place in a 100 l reactor before being transferred to the filter. After filtration, a drying oven evaporates the wet fraction to obtain the target compound. To keep the example simple, no recycling steps are included.

Next, each single process step – here the reaction step, the filtration and the drying – is calculated separately to obtain the involved material in- and output quantities (Table 6). Those values are then used to calculate the energy inputs according to the above-described equations which are summarized on Table 6. There are no fugitive emissions of volatile organic compounds since the process takes place in water.

After having scaled-up each process step singularly, the next step of the framework is to connect those including the pumping, possible (heat and/or material) recycling routes and the infrastructure of the plant. The transfer of the liquids through pumping occurs only between the reactor and the filter where the reaction mixture (m_{mix}) is transferred. Recycling of material is not feasible for this process. Although heat recovery would potentially be possible from the outlet stream of the reactor, it is not included in this example. Heat recovery from the drying oven on the other hand is already included in the efficiency. As a last step to add the contribution of the infrastructure, the amount of target compound C produced is used. With all the compiled in- and outputs of energy and material, a LCA can be performed.

3.2. Scale-dependency of the energy consumption

Investigating the change of the energy values within the various scales, shows that Q_{react} and E_{stir} do not behave linearly (Table 7), meaning that the energy consumption per kg produced decreases

Table 5
Summary of all LCA inputs and outputs.

Step	Description/Calculation	Other inputs and comments
LCA Inputs		
Reactants	Use stoichiometric amounts (same as lab protocol)	
Solvents	Reduce by 20% compared to lab scale Reduce amount by recycling rate where possible → Include energy inputs for recycling process	
Catalysts	Design recycling process where possible	
Heating	$Q_{react(1000\ l)} = \frac{\left(C_p * m_{mix} + 3.303 \frac{W}{K} * t\right) * (T_r - 298.15\ K)}{0.75}$	See Eq. (4) Secondary energy source must be chosen (electricity, fuel, gas)
Stirring	$E_{stir(1000\ l)} = 0.0180\ m^5 s^{-3} * \rho_{mix} * t$	See Eq. (6) and Table 3
Homogenizing	$E_{hom(1000\ l)} = 15.47\ m^5 s^{-3} * \rho_{mix} * t$	See Eq. (6) and Table 4
Grinding	8-16 kWh/ton	Depending on size and material
Filtration	1-10 kWh/ton dry material	Depending on grain size
Centrifugation		Centrifugation slightly higher than for filtration
Distillation	$Q_{dist} = \frac{C_p * m_{mix} * (T_{boil} - T_0) + \Delta H_{vap} * m_{dist} * (1.2 * R_{min} + 1)}{\eta_{heat} - 0.1}$	Add cooling water Heat loss included in lower efficiency
Drying	$Q_{dry} = \frac{C_{p,liq} * m_{liq} * (T_{boil} - T_0) + \Delta H_{vap} * m_{vap}}{0.8}$	
Liquid Transfer (Pumping)	$E_{pump} = 55 \frac{J}{kg} * m$	
Other Processes	Use data/values from similar existing processes or machineries	
Infrastructure	Use average dataset from *ecoinvent*: 1 unit per production plant with a lifespan of 50 years and annual output of 50′000 tons	Dataset: chemical factory construction, organics [unit]
LCA Outputs		
Reaction mixture	Output containing target compound, serves as input for subsequent step	
Product/Yield	Base yield on value of similar process or use lab yield	
Co- and By-Product	Co-product: Allocation or system expansion By-product: Allocation, system expansion or cutting out of system boundaries	
Waste	Options for solvent waste: - Recycling - Incineration on site - To hazardous waste incineration plant Other waste: - To hazardous waste incineration plant - "Regular" waste treatment if not contaminated	
Wastewater	Options for wastewater: - Recycling - Wastewater treatment plant - If contaminated: Hazardous waste incineration plant	
Emissions	Include direct emissions and estimates (use methods from Hassim et al., 2012; Hassim et al., 2010; Shine, 1996; EIIP, 2007)	
Waste heat	Include simple heat recovery through heat exchangers	

with growing scale. This becomes obvious when the respective equations are examined. In order to understand the scale-dependency, the single components of an equation need to be analyzed. The calculation of Q_{react} consists of Q_{heat} and Q_{loss} as summands in the numerator and the efficiency of the heating element (η_{heat}) in the denominator. Since Q_{heat} is obtained using either constant (C_p, T_r, T_0) or linearly-scaled (m_{mix}) parameters, it scales linearly with the size. Q_{loss} on the other hand, contains – besides constant parameters (k_a, s, T_r, T_0, t) – the geometrical measurement (A) of the reactor which does not scale linearly with its volume. Based on the geometrical calculations of a cylinder, the surface area (and consequently Q_{loss}) behaves proportionally to $V^{2/3}$, explaining a decrease in Q_{loss} at larger scales. Furthermore, also the parameter in the denominator of Q_{react}, namely the heating element's efficiency (η_{heat}), does not stay constant. Here, the efficiency is proportional to $V^{0.02}$. In the presented example, although the heat loss changes drastically with scale, it has almost no influence on the energy consumption given that Q_{heat} is orders of magnitude larger than Q_{loss}. Therefore, the change in the efficiency is practically solely responsible for the non-linear energy behavior of Q_{react}.

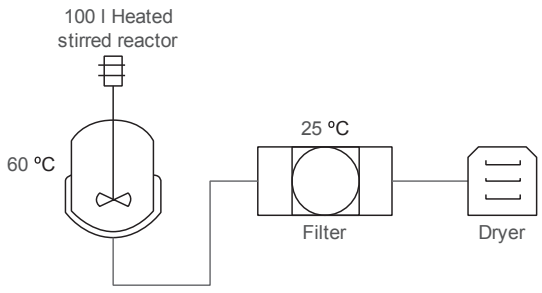


Fig. 4. Simple plant flow chart of the example reaction process.

In order to investigate the scaling behavior of E_{stir} a simple mathematical transformation of the equation is necessary. Factoring out all the constant (N_P, ρ_{mix}, t, η_{heat}) parameters, leaves two scale-dependent parameters the rotational speed (N) and the reactor's diameter (d). However, these two parameters are connected through the assumed equal tip speed, meaning that mathematical product between N and the square of the diameter is constant. Transforming the equation as shown in Equation (16) shows that the stirring energy is proportional to the reciprocal of the diameter and thus $V^{1/3}$.

$$E_{stir} = \frac{N_P * \rho_{mix} * \frac{1}{d} * (N * d^2)^3 * t}{\eta_{stir}} \rightarrow E_{stir} \propto \frac{1}{d} = \frac{1}{V^{1/3}} \quad (16)$$

Table 6
Calculation of the material in- and output for the scaled-up reaction process.

Step	Properties			Laboratory quantities					Scale-up quantities (100 l)				
Reaction step	*MW* [g/mol]	C_p [J/(kg × K)]	ρ [g/cm^3]	*Eq.*	*n* [mmol]	*m* [g]	*V* [cm^3]	ρ [g/cm^3]	*Eq.*	*n* [mol]	*m* [kg]	*V* [m^3]	ρ [kg/m^3]
Reactant A	174			1	5	0.87			1	2.5	0.435		
Reactant B	66			2	10	0.66			2	5	0.330		
H_2O (solvent)	18	4181	1	2778 (100%)	13.89 k	250	250		2222 (80%)	5556	100	0.1	
Catalyst	380			0.001	0.005	0.0019			0.001	0.0025	0.95 g		
Reaction mixture						251.532	250	1.006			100.77	0.1	1008
Q_{react}									5.76 kWh				
E_{stir}									0.007 kWh				
Filtration													
Reaction mixture						251.532	250	1.006			100.77	0.1	1008
Filtrate – hazard. waste						250.029					100.01		
Filtercake (wet fraction)						1.503 (5.33%)					0.752 (5.33%)		
E_{filt}									0.55 kWh				
Drying													
H_2O to air		4181				0.080					0.040		
Product C	153			1.86 (93%)	9.3	1.423			1.86 (93%)	4.65	0.711		
E_{dry}									0.036 kWh				
E_{pump}									0.0015 kWh				
$unit_{infrast}$									2.85×10^{-10} units				

Table 7
Scale-dependency of calculated energy values.

Step	100 l	500 l	1′000 l	5′000 l	10′000 l
Reaction step					
Q_{heat} [kWh]	4.10	20.48	40.96	204.80	409.60
% of linear scaling	100%	100%	100%	100%	100%
Q_{loss} [kWh]	0.050	0.146	0.231	0.676	1.073
% of linear scaling	100%	58.47%	46.41%	27.14%	21.54%
$1/\eta_{heat}$	1.39	1.35	1.33	1.30	1.27
% of constant scaling	100%	97.30%	96.00%	93.51%	91.14%
Q_{react} [kWh]	5.76	27.87	54.92	266.85	519.84
% of linear scaling	100%	96.81%	95.38%	92.69%	90.28%
E_{stir} [kWh]	0.007	0.021	0.033	0.096	0.151
% of linear scaling	100%	58.67%	46.63%	27.24%	21.59%
Filtration					
E_{filt} [kWh]	0.55	2.77	5.54	27.71	55.42
% of linear scaling	100%	100%	100%	100%	100%
Drying					
E_{dry} [kWh]	0.036	0.179	0.357	1.787	3.574
% of linear scaling	100%	100%	100%	100%	100%

4. Discussion and conclusion

The scale-up framework is relatively simple and applicable without the need of an advanced knowledge in the field of chemical engineering, as shown in the example, while still delivering valuable results. The focus on laboratory-scale processes is a key feature, as it covers an area of research that has been largely neglected so far. The scale-up framework allows to obtain a first estimate about the (future) impacts of the material production at an industrial scale and thus, improves the comparability with commercially available products.

The proposed framework offers a selection of common processes from wet chemistry. By analyzing these frequent processes in wet chemistry, we developed certain relevant factors – ranging from elaborate calculation procedures to qualitative guidance - to facilitate the LCA scale-up of lab experiments to an industrial scale. However, the calculations do not represent exact values but rather logical and quantitative estimates. This is especially true for the steps resulting in high relative contribution. In chemical engineering, each step involves several and complicated calculations and decisions. For each of these, there are multiple options. This can have a large impact on the final LCA results. Scenario analyses are therefore an important and decisive aspect for the robustness and credibility of a scale-up study.

Decisions in the design of a chemical production plant are usually driven by economic motivation opposed to environmental criteria. In the event of a trade-off between a cost efficient and an energy saving process, the former will presumably be chosen. This economic reasoning is difficult to reflect in the simple theoretical design of a production plant as proposed for this framework. However, beyond the results of the environmental impacts, this scale-up framework offers further advantages: simple estimations of the variable production costs become possible. The obtained in- and output values for the LCA can be translated into costs, meaning that the research can already be adapted to obtain a higher degree of cost competitiveness.

The limitations or open points of the approach mainly regard its limited applicability and the data quality. The presented framework is limited to heated liquid phase batch reactions and certain isolation, purification and processing steps. Other processes, such as continuous or semi-batch, and reactions (e.g. solid state, gas phase, solid–liquid etc.) are not included so far. Furthermore, future technologies are not included, restricting the processes to existing techniques. This means that the scale-up of a new process step is not possible with this framework unless a similar step is already used at an industrial scale. Because it follows an engineering based theoretical approach, it does not include empirical data, which would validate the technique and provide values for the uncertainty and reliability of the results. Given the predictive nature of a scale-up simulating a possible future production plant, it includes several assumptions about the future which contain a high degree of uncertainty. The results of the scale-up depend on the knowledge and the data quality that is applied, scaling the process approximately using the same steps as in the laboratory scale. Hence, only limited experience effects (i.e. process optimization that come along with the experience after use during an extended period of several years) are included to reflect the improvement of the efficiency that does not derive from the change of scale. Consequently, it is extremely important to include scenario analyses in the scale-ups to understand the implications of assumptions and manage the uncertainty. However, this proposed scale-up

framework is a first approach to deliver critical data, helping to improve chemical processes from mainly an environmental but also an economic perspective.

The framework is not an alternative for developed methods by other researchers. It is a complementary approach, which adds another dimension in the scale-up of chemicals processes for LCA studies, addressing earlier points of development. We consider it the best approach available when the research is still at the laboratory stage. In contrast to average empirical data, it offers the opportunity to assess and display the process on case specific data. With that information, an additional dimension for the analysis is displayed, e.g. by showing the impact of substituting a specific solvent.

Assessing environmental impacts using conservative assumptions means that the likely results will be higher than what is potentially achievable, assuring that it is not underestimated. Although this might weaken the potential of the technology, the approach of overestimation is favorable for environmental assessments. Hasty conclusions can be avoided and it is preferable, in our opinion, to explain the deviation than obtaining values that ultimately cannot be achieved. As there are many assumptions and simplifications involved, it is of pivotal importance for the credibility of the study to maintain a high transparency when a scale-up is performed and to include scenario analyses for the most important steps.

The presented framework is a useful approach to perform an industrial scale LCA of a production process that has not passed beyond the laboratory experiments yet. The results obtained from such a scale-up give a first approximation of possible environmental impacts related to this material. An opportunity is thus opened to compare a new production process to competing materials that are already on the market and produced at an industrial scale. Additionally, it helps to assess the process itself by highlighting hotspots and bottlenecks with high contribution to the environmental impact. In certain cases, those are not the same as if the lab scale production would be assessed. This helps to improve the production process in perspective of a possible production plant before even a mini or pilot plant has been installed.

A scale-up based on the laboratory experiments might be useful in justifying the research of a new material or process by showing its potential environmental performance. Further application and development will help in optimizing the results and the procedure of this framework and an expansion to more processes (e.g. continuous reactions, inclusion of gaseous and solid state reactions, cooling etc.) is desirable. The framework has a high degree of practicality helping in research projects to show and improve the sustainability of new chemistries and materials. Allowing more meaningful comparative LCAs, the developed framework can also support the justification and further development of new technologies.

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