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PAPER

# Decision support towards agile eco-design of microreaction processes by accompanying (simplified) life cycle assessment

**Sabine Huebschmann,[a] Dana Kralisch,*[a] Holger Loewe,[b,c] Denis Breuch,[b] Jan Hauke Petersen,[b] Thomas Dietrich[d] and Ralf Scholz[d]**

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Continuously running syntheses in microstructured reactors offers novel ways to intensify conventional chemical processes. An outstanding advantage of microreaction technology is the high surface-to-volume-ratio which enables intensive mixing phenomena as well as high mass and heat transfer rates. Thus, microstructured reactors may be a suitable means to improve multiphase reactions by increasing the interfacial area and the intensification of internal mixing. This improvement in reaction performances may lead to reduced environmental burdens of the process under consideration. The method of simplified life cycle assessment (SLCA) is a suitable tool to evaluate the environmental burdens caused by chemical processes. It has been applied already in research and development to identify the key parameters for a deliberate green process design of two biphasic reactions, the esterification of phenol and benzoyl chloride resulting in phenyl benzoate and the synthesis of one of the corresponding phase transfer catalysts, [BMIM]Cl. Further, SLCA is complemented by a simple cost estimation to investigate the main cost drivers relevant for possible industrial application of the syntheses investigated.

## Introduction

The need to create more sustainable processes, to use raw materials more efficiently and to save energy as well as money has become an important issue in the chemical industry. Several concepts have been developed to reduce the environmental burdens of chemical processes, *e.g.*, by implementing catalysts, substituting petrochemical substances by renewable feedstocks, employing alternative energy sources or implementing novel reaction media. Another possibility to obtain more sustainable processes is the intensification of the process itself which can be achieved, *e.g.*, by the transmission of conventional batch processes to continuously running processes in microstructured reactors while maintaining or improving the reaction yield and/or selectivity.[1–3]

Due to there inherent large surface-to-volume ratio, which may lead to intensive mixing as well as to very efficient mass and heat transfers, microstructured reactors are gaining increasing interest not only in academic but also in industrial applications. Further, hazardous and toxic substances can be handled more safely because of the small inner volumes of the reaction channels. A high flexibility is obtained by the modular assembling of the microreactor plant including pumps and controlling instruments.[4] The residence times can be precisely adapted to the reaction under investigation by controlling the flow rates to avoid side and subsequent reactions.[5]

Phase transfer catalyses are often difficult to handle in conventional reactor equipment, because these reactions are mostly mass transfer controlled, requiring a high and reproducible interfacial area. In microstructured reactors, an increased and well-defined interfacial area is achieved by realizing a segmented flow.[6,7] Further, the internal mixing of reactants can be increased by a circular flow within the single plugs of the dispersed phase. A dispersion as well as a coalescence of both immiscible fluids can be minimized by regular-sized individual plugs in a continuous phase.[8,9]

However, there may also be some difficulties in handling multiphase reactions in microstructured reactors. For example, the flow rates have to be precisely adapted to the system under investigation. This also includes the flow rate ratios of the process fluids in order to avoid parallel flow of both fluids, which decreases the interfacial area and the mass transfer.[7]

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[a] *Institute of Technical Chemistry and Environmental Chemistry, Friedrich-Schiller-University Jena, D-07443, Jena, Germany. E-mail: dana.kralisch@uni-jena.de; Fax: +49-3641-9484-02; Tel: +49-3641-9484-57*

[b] *Institute of Organic Chemistry, Johannes Gutenberg University Mainz, Duisbergweg 10-14, D-55128, Mainz, Germany. E-mail: loewe@uni-mainz.de; Fax: +49-6131-392-6677; Tel: +49-6131-392-6667*

[c] *Institut fuer Mikrotechnik Mainz GmbH, Carl-Zeiss-Str. 18-20, D-55129, Mainz, Germany*

[d] *mikroglas chemtech GmbH, Galileo-Galilei-Str. 28, D-55129, Mainz, Germany. E-mail: T.Dietrich@mikroglas.com; Fax: +49-6131-55550-52; Tel: +49-6131-55550-50*

Furthermore, even small fabrication defects may lead to a completely different flow behaviour.[10] Since continuously operating devices for the separation of two liquid–liquid phases are still under development, there may also be some difficulties in separating both phases after the reaction as well as in the isolation of the product.[11–14]

Nevertheless, the continuous processing of phase transfer catalysis in microreactors bears the potential for significant yield enhancements and reductions in energy requirements which may lead to more sustainable chemical processes compared to conventional reaction equipment. This has been proven in the examples of the phase-transfer catalysed phenyl benzoate synthesis starting from phenol and benzoyl chloride. Several ionic liquids have been tested as phase transfer catalysts for this reaction. Thus, they were included in the comparative evaluation of the resulting environmental and cost impacts. Exemplarily, the synthesis of the ionic liquid [BMIM]Cl from 1-methylimidazole and butyl chloride will be discussed in more detail, since the benefits of microprocessing for biphasic reactions have become visible here as well. In both cases, an accompanying simplified life cycle assessment (SLCA) and cost estimation approach gave the direction for a deliberate design of a green chemical process.

In the past decades, several metrics and concepts have been developed to evaluate the environmental burdens of a product or process, *e.g.*, the E-factor by Sheldon,[15] the concept of atom economy by Trost,[16] EATOS by Eissen and Metzger[17] as well as E-Green by Hossain *et al.*[18] However, the most comprehensive method is the life cycle assessment (LCA) standardized in the ISO norms 14040[19] and 14044.[20] According to these norms, the whole life cycle of a product or process from the extraction of raw materials, the manufacture or synthesis of the product until the use and disposal are to be investigated. In the first step, the boundaries of the system under investigation and the functional unit are defined. Afterwards, all mass and energy flows within the system boundary are comprehended referring to the functional unit (life cycle inventory analysis – LCI) and the environmental impacts of these mass and energy flows are assessed (life cycle impact assessment – LCIA). In the last step, all results are summed up and interpreted to derive potential improvements or to support decisions between different options.

Usually, LCAs are performed at the end of process development because detailed information of the process under investigation is required according to the ISO norms. This information is often not sufficiently available during research and development (R&D) stages. Data gaps and uncertainties are typical problems during this stage of process design and impede a sufficient evaluation. Further, R&D stages are regarded as making only a minor contribution to the overall environmental impact of a process.[21] But environmental burdens of a process become mostly predefined by the decisions made during R&D and high efforts are required to reduce these impacts subsequently.[22–24] Thus, several authors[25–27] have already pointed out that evaluation methods most beneficially are applied during R&D. To address the environmental burdens in these early stages of process development, qualitative criteria have been proposed by Anastas and Warner,[28] Anastas and Zimmerman,[29] Biwer and Heinzle,[22] as well as by Graedel.[30] Several quantitative metrics have also been developed going into further detail, *e.g.*, euroMat by Fleischer and Schmidt,[24] the MIPS concept,[31] the EHS method by Koller*et al.*[32] or an algorithm proposed by Sugiyama *et al.*[33] starting with an estimation based on stoichiometry and becoming more detailed with every iteration step. The latter approach introduced also the ELI (energy loss index) as a new indicator for estimating energy costs in early process design, which was further refined by Bumann *et al.*[34] Some authors have also suggested the combined evaluation of environmental burdens and process costs during R&D, *e.g.*, the ECO method proposed by Kralisch*et al.*,[25] as well as a combination of the environmental indicator MIPS and an economic parameter TAPPS suggested by Hoffmann *et al.*[35]

We have found that a simplified LCA (SLCA) provides a suitable compromise between single metrics and a holistic life-cycle-based analysis, which provides an insight into the environmental impacts of a chemical process under development and for decision support between several alternative reaction pathways. SLCA can either comprise simple input/output analyses or hybrid analyses, but may also consist of a horizontally limited approach by neglecting some life cycle stages. But, a horizontally limited approach may lead to a problem shift to the life cycle stages not taken into consideration.[21] Because of this, vertically bounded SLCA, which consider all life cycle stages but in a superficial manner, are more recommended. These SLCA approaches are regarded as suitable for screening purposes[36] as they are less cost- and time-consuming than detailed LCAs.[37]

In the following, a research accompanying SLCA is described. It has been performed in order to evaluate the environmental burdens of the continuously running phase transfer catalysis of the biphasic esterification of benzoyl chloride and phenol resulting in phenyl benzoate in microstructured reactors, which already starts in research and development stages. We also applied this method to the biphasic synthesis of the ionic liquid [BMIM]Cl in laboratory scale carried out both in batch as well as in continuously running syntheses. Further, the costs of the syntheses in laboratory scale were estimated to predict the economic competitiveness of the reactions under investigation compared to the actual market price. The main cost drivers of the syntheses and thus the key figures for process improvement could be identified by this approach.

## Evaluation approach

In this section, the applied methods for performing the SLCA as well as for cost estimation are described. The strategy for research accompanying environmental as well as economic assessments are illustrated in Fig. 1. As we had already successfully applied it in other case studies, we started our investigations with SLCA during R&D, when the knowledge about the process was still very low.

During process design there are vast amounts of process alternatives to choose from. Thus, scenario analyses have been performed to support the decisions regarding these alternatives. Additionally, sensitivity analyses were used to identify parameters with major influences on the environmental impact of the process. At the end of process development, when the system is known in detail, a holistic LCA will be performed to validate the decisions taken. During all process development stages, the costs were also considered, again starting already at the laboratory scale. The results were adapted according to

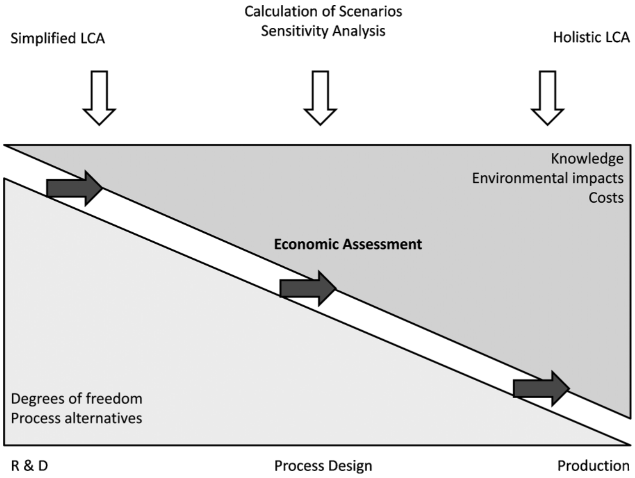


**Fig. 1** Beneficial application of evaluation methods during process development.

the knowledge about the process obtained during experimental work, which was performed mainly at the Johannes-Gutenberg-University Mainz, to identify major environmental hot-spots and cost drivers.

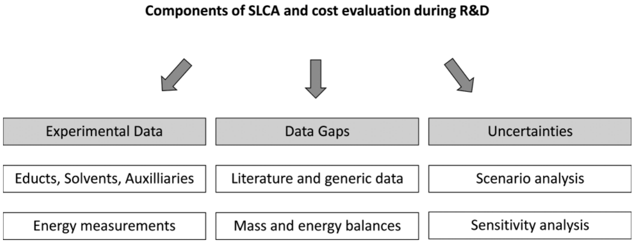
## Simplified life cycle assessment

We decided to evaluate the environmental burdens of the processes under investigation by a vertically bounded SLCA,[21] including all life cycle stages from source to gate to avoid problem shifts to down-stream processes. For this, we followed the desimplification approach proposed by the Society of Environmental Toxicology and Chemistry (SETAC Europe).[37] These assessments were performed in accordance to the ISO norms 14040 and 14044.

Frequently occurring data gaps, which are inherent to R&D stages, may occur, for example, when:

- reaction yields are directly analyzed from the reaction mixture without the application of work-up procedures;
- the energy consumption is not measured;
- only major solvent fractions are recycled, whereas smaller amounts of catalysts or solvents are mostly disposed.

In our approach, these data gaps were overcome by the hypothetical calculation of work-up procedures and the completion of experimental data by generic data which enabled the performance of mass and energy balances (Fig. 2). The assessments are refined iteratively by close collaboration with the researchers in the laboratory as more and more experimental data become available. Scenario-based calculations as well as sensitivity analyses were performed by varying significant parameters, *e.g.*, the amount of solvents used, the reaction yield, the type of micromixer or the flow rates.



| Experimental Data | Data Gaps | Uncertainties |
|---|---|---|
| Educts, Solvents, Auxilliaries | Literature and generic data | Scenario analysis |
| Energy measurements | Mass and energy balances | Sensitivity analysis |

**Fig. 2** Components of SLCA and cost evaluation during process development.

We chose Umberto[38] as the software tool for process modelling during life cycle inventory (LCI) analysis and for the implementation of the life cycle impact assessment (LCIA). The Ecoinvent[39] database was used to account for the up-stream processes of the substances involved as well as the generically calculated supply of electrical energy. The environmental burdens of the process alternatives were assessed by means of the cumulative energy demand (CED)[40] as well as the life cycle impact categories proposed by CML.[41] By this, the environmental burdens of the up-stream processes of the supply of the substances involved in the syntheses, the syntheses itself and the recycling of the organic solvents were investigated.

As the experimental work in the phase transfer catalytic synthesis of phenyl benzoate is still going on, no work-up procedures have been applied yet. Nevertheless, we made some prognostic calculations to guide further process design, since the work-up procedures may have a significant influence on the overall SLCA result. In many cases, the efficiency of the work-up procedure decides the superiority of one process alternative against others. In the synthesis of [BMIM]Cl, two work-up procedures were established depending on the processing mode, which were fully included in the SLCA investigations as well as in the cost estimation. However, the provision of the reaction periphery is not included in the environmental evaluation, because a previous study[42] showed that the environmental burdens of the technical equipment are only of minor importance.

Before the establishment of a suitable reaction set-up for microreaction processes, some batch syntheses are usually conducted as internal benchmarks. Afterwards the reaction is transferred to the microreactor plant, where several process alternatives are tested and optimized during the ongoing process development. Thus, the batch syntheses as well as the continuously running processes have been evaluated by SLCA in both case studies and the results of these screenings were compared with each other to derive further optimization potential.

## Economic evaluation during process development

Conjointly to the SLCA investigations, a screening concerning economic hot-spots has been performed. In case study 1, the costs of one batch reaction as well as the continuously running processes were estimated based on the reaction protocols. Furthermore, information about manpower requirements as well as the investment and maintenance costs for the reactor equipment were included in the estimation. All costs were estimated at laboratory scale.

Although these costs are significantly higher than the actual market price of the product, the comparison should be performed on one scale.

The general method applied was as following:

(1) calculation of annual production capacities based on reaction yields;

(2) calculation of annual material and energy costs based on the annual production capacities;

(3) determination of the annual investment and maintenance costs based on a 10 year period;

(4) calculation of annual labour costs based on annual production capacities;

(5) summation of all costs on an annual basis and assessment of total costs per kg of product.

As the microreactor plant operates fully automatically, stopping only in case of a disaster, the annual operating time was calculated on the basis of 350 days per year and 24 hours per day. Contrary to the continuously running reactions, the batch processes can only be conducted under permanent attendance of a laboratory assistant. For the sake of comparability between both processing modes, we assumed a three-shift operation for the batch reactions which can also be realized by the operation of 3 batch reaction set-ups at one time. Thus, 6000 working hours per year were considered for the batch process. Additional to the mere reaction times, a cleaning procedure carried out once a week was assumed in the case of the continuously running reactions as well as a cleaning procedure after each batch reaction.

The material and energy costs were calculated based on the reaction protocols linearly extrapolated to the annual production capacity of each scenario considered. Current catalogue prices as well as prices for electricity and water were used to estimate the annual material and energy costs.

A lifetime of 10 years was assumed for the microreaction plant although not all components were considered to work all this time. Thus, components with a shorter lifetime were considered to be replaced during the 10 year period. The current market prices of these components were added to the investment costs of the microreactor plant itself. These total investment costs were divided by 10 according to a usual depreciation period. Additionally, the annual maintenance costs were included in these fix costs.

In the case of the batch synthesis, we considered standard laboratory equipment consisting of round bottom flasks, magnetic stirrer with heating function, mechanical stirrer, and reflux condenser. The purchasing costs of these items were also calculated to a 10 year period taking under consideration the (estimated) lifetime of every item.

In the next step, the labour costs were calculated based on the annual operation time of the continuously running processes. Further, the gross hourly labour costs of a laboratory assistant were estimated, including the employer's contribution to social insurance.

Finally, all these costs were summed up on an annual basis and related to 1 kg of product.

As the purpose of the cost estimation was a relative comparison of main cost drivers in batch and continuously running syntheses, we did not consider any inflation rates which may affect the estimation of fixed costs during the 10 year period. Further, we did not estimate any fluctuations in substance prices or variations in labour costs which may be due, for example, to legal measurements or salary adjustments.

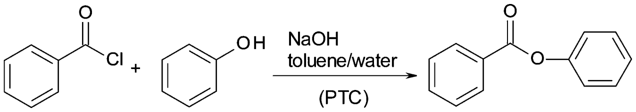
Cost estimation for the adaptation of the developed processes to industrial scale were based on the reaction protocols already applied for cost estimation in laboratory scale. The amounts of substances used were extrapolated to typical industrial production capacities (1000 tons per year) and multiplied with prices for large purchase quantities.[43]

We decided not to perform cash flow analyses or to calculate return on investment, since this would also require the consideration of cost fluctuations.

The proposed method for cost estimation in laboratory scale was also applied to case study 2. For calculation of fixed costs of the continuously running syntheses, we considered the same microreactor plant as in case study 1.

## Case study 1: synthesis of phenyl benzoate

As mentioned above, multiphase reactions may be carried out beneficially in microreactors. Thus, the phase transfer catalysis of phenol and benzoyl chloride giving phenyl benzoate (Scheme 1) was investigated by means of SLCA and cost estimation. Phenyl benzoate is an industrially relevant chemical substance, which is used for polymer modification and as an anti-oxidant,[44] as well as an intermediate in the production of liquid crystals.[45] The continuously running reactions were performed utilizing micromixers with different mixing structures and partly applying ionic liquids as phase transfer catalysts.



**Scheme 1** Phase transfer catalysis of benzoyl chloride and phenol giving phenyl benzoate.

The experimental data used in the research accompanying economical and ecological assessments were provided by the working group of H. Loewe at the Johannes-Gutenberg-University Mainz, Germany. All continuously running processes where performed in a microreaction plant designed by mikroglas chemtech GmbH, Mainz, Germany. This lab bench scaled plant was custom-designed in close collaboration with Loewe and coworkers to meet the needs of multiphase reactions.

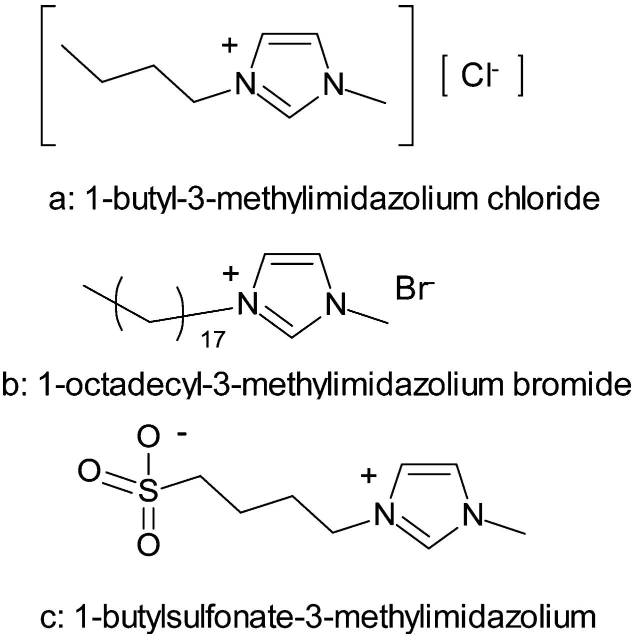
Two batch syntheses, without a catalyst and with the ionic liquid [BMIM]Cl in catalytic amounts, were evaluated by SLCA to establish an internal benchmark. These two experiments already revealed the phase transfer catalytic potential of ionic liquids.

The continuously running experiments in the microreactor plant were carried out to investigate the influence of increasing the interfacial area by different micromixers (interdigital mixer, herringbone structured mixer and emulsification mixer), which were also provided by mikroglas chemtech GmbH. These glass micromixers were used to generate uniform microbubbles while simultaneously enabling a precise determination of the interfacial area. Due to the mixing structure chosen, the residence times differed from 0.83 s to 1.355 s. The reaction conditions investigated are summarized in Table 1. The only side reaction which may occur in the syntheses of phenyl benzoate from benzoyl chloride and phenol is the hydrolysis to benzoic acid. But, as the reaction solution was analyzed both by IR spectroscopy and gas chromatography the amount of side product was always less than 1%.

As phase transfer catalysts, the ionic liquids [$C_{18}$MIM]Br and [MIM]Bu$SO_3$ were used in the continuously running syntheses (Scheme 2). In the batch synthesis, [BMIM]Cl was implemented as a phase transfer catalyst. The three ionic liquids used in the

**Table 1** Reaction conditions used for SLCA investigating the phase transfer catalysis of phenol and benzoyl chloride giving phenyl benzoate

| Entry | Catalyst | $T/°C$ | Mixing structure | Residence time [s] | Yield [%] |
|---|---|---|---|---|---|
| 1 | No catalyst | 57 | Interdigital mixer | 0.83 | 10 |
| 2 | No catalyst | 57 | Herringbone mixer | 18.8 | 26 |
| 3 | $[C_{18}MIM]Br$ | 62 | Herringbone mixer | 18.8 | 45 |
| 4 | $[C_{18}MIM]Br$ | 68 | Emulsification mixer | 1.355 | 51 |
| 5 | $[C_{18}MIM]Br$ | 75 | Interdigital mixer | 0.83 | 62 |
| 6 | $[MIM]BuSO_3$ | 30 | Interdigital mixer | 0.83 | 70 |
| 7 | No catalyst | 66 | Batch synthesis | 5400 (90 min) | 66 |
| 8 | [BMIM]Cl | 45.5 | Batch synthesis | 2700 (45 min) | 72 |



**Scheme 2** Ionic liquids used as phase transfer catalysts: (a) [BMIM]Cl, (b) $[C_{18}MIM]Br$, (c) $[MIM]BuSO_3$.

reactions as phase transfer catalysts were synthesized in the working group of H. Loewe in the following procedures:

A continuously running microreactor plant provided by the Institut für Mikrotechnik, Mainz, (IMM) was used to synthesize the ionic liquid [BMIM]Cl from 1-methylimidazole and butyl chloride (5% molar excess) at 145 °C and 6 bar. The product was obtained by distillation of non-reacted butyl chloride and recrystallization of the crude product from acetone.[46] As the neat reaction of butyl chloride and 1-methylimidazole is also a biphasic reaction, the synthesis of [BMIM]Cl is subject to case study 2.

$[C_{18}MIM]Br$ was obtained by reacting equimolar amounts of octadecyl bromide and 1-methylimidazole in a round bottom flask for 48 h at 90 °C. Afterwards the crude product was recrystallized from tetrahydrofuran.[10]

As the synthesis of $[MIM]BuSO_3$ is highly exothermic, the reactants 1-methylimidazole and 1,4-butane sulfone were premixed in a T-junction *in situ* dropped into hot vapors of toluene. By this method, no further work-up was needed to purify the ionic liquid after the distillation of toluene, since toluene also functions as a recrystallization medium.[10]

The energy consumed during the reaction was estimated based on thermodynamics both for batch syntheses as well as for continuously running reactions. Here, an efficiency of heat transfer under laboratory conditions of 40% (based on experimental studies) was assumed. In contrast, the energy consumption of the periphery in the case of the continuously running syntheses, *e.g.* pumps and control systems, were based on measurements.

As the process design is still under development, there has not yet been a work-up procedure applied, since the reaction yields were analyzed directly from the reaction mixture by gas chromatography. Thus, we considered the recycling of the organic solvent toluene by assuming a redistillation and estimated the energy consumption by using thermodynamic data. This was completed by the calculation of two (hypothetical) scenarios for the work-up of the reaction mixtures in microreactors including ionic liquids as catalysts (entries 5 and 6). Here, we considered a phase separation (in batch mode) first. The product remained in the organic phase and was washed several times and dried over sodium sulfate. Afterwards, the toluene was removed by distillation since the boiling point of phenyl benzoate (315 °C) is much higher than that of toluene (111 °C). The ionic liquids as well as non-reacted benzoyl chloride (as sodium benzoate by reaction with sodium hydroxide) and phenol are soluble in the aqueous phase and can be separated easily from the product.

In order to avoid disposal problems for the contaminated aqueous phase due to the remaining ionic liquid and non-reacted reactants, we assumed a distillation of the water and a disposal of the residual organic substances including ionic liquid as organic waste

## Results

The functional unit chosen for both the SLCA as well as the economic evaluation was 1 kg of the product phenyl benzoate. All results are related to this unit.

### Simplified life cycle assessment

We investigated the environmental burdens of the process simultaneously during the ongoing process development by the SLCA approach mentioned above. By this method, the continuously running syntheses were compared to the reference batch syntheses with and without the implementation of a phase transfer catalyst.

By means of the SLCA we addressed the following questions:

*I. Are the continuously running syntheses more environmentally benign than the batch syntheses?*

*II. What is the influence of the periphery in the energy consumption of the continuously running syntheses compared to the batch reactions?*

*III. Is the higher yield obtained by the implementation of ionic liquids as phase transfer catalysts compensated by higher environmental burdens caused by the supply of the ionic liquids?*

*IV. Which mixing structure is the most efficient?*

*V. Which ionic liquid is more beneficial from an ecological point of view?*

*VI. How does the consideration of work-up procedures affect the environmental burdens of the process?*

In Fig. 3 some toxicity potentials proposed by CML[41] are shown, presenting the most environmentally benign scenarios in the centre of the chart.

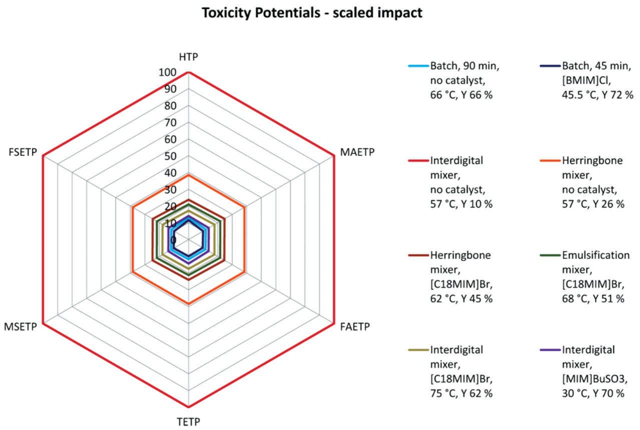


**Fig. 3** Overview of various toxicity potentials of the biphasic reaction of benzoyl chloride and phenol giving phenyl benzoate (HTP – human toxicity potential, MAETP – marine aquatic ecotoxicity potential, FAETP – fresh water aquatic ecotoxicity potential, TETP – terrestrial ecotoxicity potential, MSETP – marine sedimental ecotoxicity potential, FSETP – fresh water sedimental ecotoxicity potential).

The highest toxicity potentials are caused by the continuously running synthesis in an interdigital mixer without the implementation of a phase transfer catalyst (entry 1). These environmental impacts of the uncatalyzed reaction can be reduced significantly by substituting the interdigital mixer with a herringbone structured mixer (entry 2). Because of its considerably higher environmental burdens, entry 1 was used as a reference for scaling the environmental impacts. For the sake of better clarity, in Fig. 4 further environmental impacts are presented without the indication of entry 1. Here, a strong reversed correlation between reaction yields obtained and the resulting environmental impacts is observed due to less process waste and a more efficient use of materials and energy.

In the following, the human toxicity potential (HTP) and the global warming potential (GWP) as well as the cumulative energy demand (CED) are chosen for a more detailed analysis of environmental impacts. The HTP reflects emissions of the process under investigation including up-stream processes which are harmful to human health due to acute or chronic toxicity as well as cancer-causing effects.

As can be seen from Fig. 5, the supply of phenol as well as the energy consumption of the periphery in the continuously running syntheses give the highest contribution to the HTP. Further, reactions without the implementation of a phase transfer catalyst (entries 1 and 2) reveal a higher HTP than the reactions implementing ionic liquids. However, a reduction of the HTP by more than 60% in the case of the uncatalyzed continuously-running reaction can be obtained by simply substituting the interdigital mixer by the herringbone-structured mixer. In contrast, the interdigital mixer performed best under phase-transfer catalytic conditions.

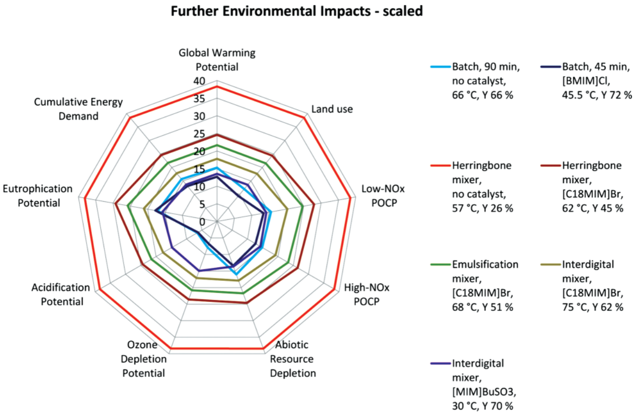


**Fig. 4** Further environmental impacts of the biphasic reaction of benzoyl chloride and phenol giving phenyl benzoate (POCP – photochemical ozone creation potential).

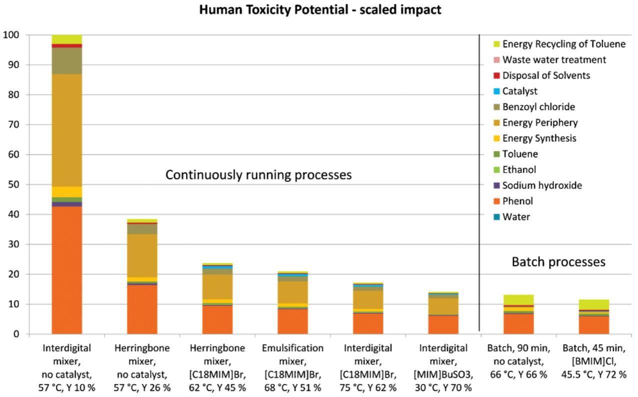


**Fig. 5** HTP of the biphasic reaction of benzoyl chloride and phenol giving phenyl benzoate.

The GWP indicates the greenhouse gas emissions caused by the process as well as the up-stream processes. In Fig. 6, presenting the GWP, the same trends as in the analysis of the HTP could be observed. But, the energy consumed by the periphery of the continuously-running processes during the reaction exhibits the highest influence.

In both impact categories, the lowest environmental impacts of the continuously-running phase transfer catalysis are caused by the reaction in the interdigital mixer implementing [MIM]BuSO$_3$ (entry 6).

This reaction is conducted at 30 °C resulting in a low energy demand for the reaction itself, which is mostly consumed by the plant periphery. Surprisingly, the ionic liquids have only a minor influence on the environmental impact, which is counterbalanced by the significantly higher reaction yields obtained in the catalyzed reactions. This is opposite to other investigations where the environmental impacts were dominated

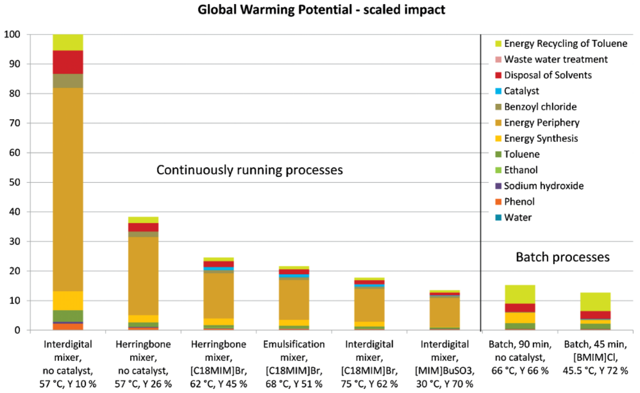


**Fig. 6** GWP of the biphasic reaction of benzoyl chloride and phenol giving phenyl benzoate.

more or less by the supply of these compounds if they were used as a solvent in chemical syntheses.[26,47,48] However, in the reactions discussed here, [BMIM]Cl, [$C_{18}$MIM]Br and [MIM]$BuSO_3$ were implemented only in catalytic amounts instead of being used more commonly as solvents. Nevertheless, [MIM]$BuSO_3$ has been found to be more beneficial from an ecological point of view than [$C_{18}$MIM]Br, because it is synthesized in an exothermic reaction, whereas the latter one is obtained after 48 h of heating to 90 °C. But, [BMIM]Cl used in the batch synthesis reveals the lowest overall environmental impacts due to its plain reactants and the easy synthesis, as can be seen from Fig. 7. Merely in the impact categories Ozone Depletion Potential and Terrestrial Ecotoxicity Potential, the environmental burdens of [MIM]$BuSO_3$ exceed that of [$C_{18}$MIM]Br.

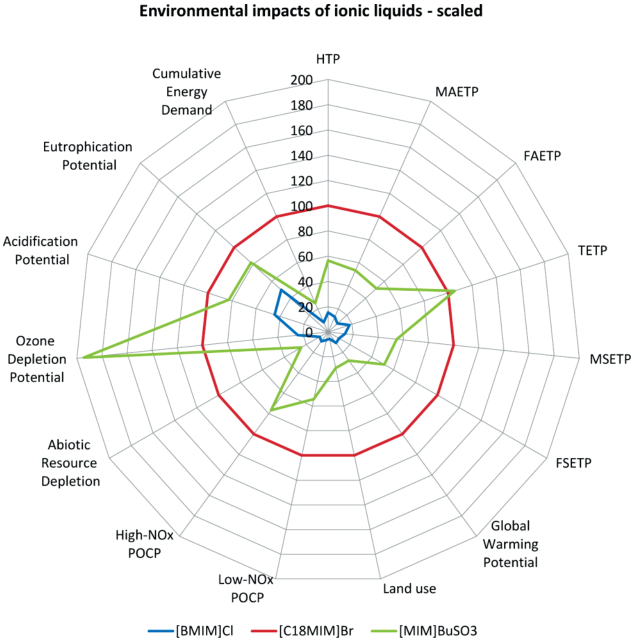


**Fig. 7** Overall life cycle impacts for the three ionic liquids implemented as phase transfer catalysts.

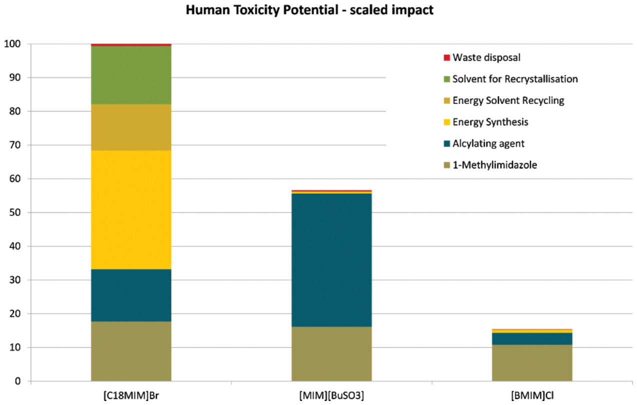


**Fig. 8** HTP for the syntheses of the three ionic liquids used as phase transfer catalysts.

The result of lower environmental impacts caused by [BMIM]Cl in comparison to [$C_{18}$MIM]Br and [MIM]$BuSO_3$ can also be confirmed by Fig. 8, which exemplarily shows the HTP of the ionic liquid syntheses. It can be seen from this figure that the environmental burden of the supply of [$C_{18}$MIM]Br is mainly caused by the energy consumption during the reaction. Against this, the HTP of [MIM]$BuSO_3$ is mainly caused by the provision of the acylating agent 1,4-butane sulfone. Please pay attention to the fact that, contrary to the comparison of the alternative reaction procedures of the phase transfer catalysis on a kilogram scale, the ionic liquids were compared on a molar basis as the catalysts were added to the reaction mixture in a fixed molar amount.

Further we found that the batch syntheses with and without the implementation of a catalyst (entries 7 and 8) show similar environmental impacts as the continuously running processes implementing [$C_{18}$MIM]Br or [MIM]$BuSO_3$ under the employment of an interdigital mixer (entries 5 and 6) in all impact categories (Fig. 3–6). This results from the energy demand of the plant periphery in the continuously-running syntheses which reveals a considerable impact on the environmental burdens of the processes.

In contrast, the batch reactions can be carried out without any energy for pumping or controlling at the laboratory scale. However, this apparent advantage of the batch processes is suppressed when the processes are transferred to the industrial scale. At industrial scale processing, pumps and controlling instruments are needed for both continuously running as well as batch reaction processing modes. To illustrate this issue in more detail, the CED for the continuously running esterification with the implementation of [$C_{18}$MIM]Br and [MIM]$BuSO_3$ (entries 5 and 6) is shown in Fig. 9. The CED comprises all energy consumed during the whole processing chain from the supply of raw materials and electrical current, the reaction itself, as well as the work-up and the disposal of wastes. In this figure the continuously running syntheses are presented both, with the consideration of the energy demand of the plant periphery and without its consideration. These results are opposite to the CED of the batch syntheses (entries 7 and 8) indicating, that under similar conditions, *i.e.* under the same energy demand for pumping and controlling, the continuously running syntheses would be 2 to 3 times more beneficial from an ecological point of view (see also Huebschmann *et al.*[49]).

Although no experimental work has been performed so far to introduce an efficient work-up procedure of the ionic liquids

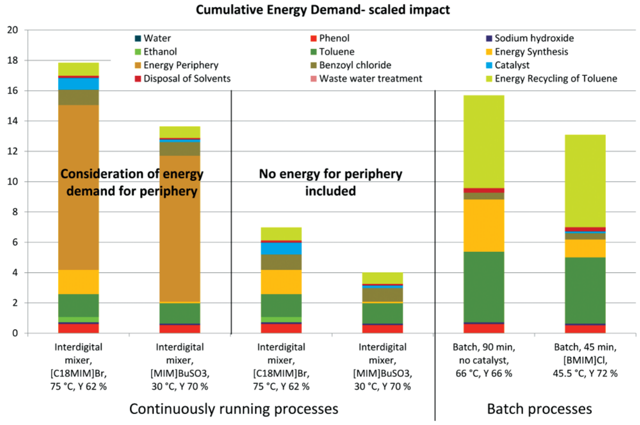


**Fig. 9** CED for the continuously running biphasic reaction of benzoyl chloride and phenol under consideration of the energy needed by the reaction periphery (left) and without the consideration (middle) *vs.* the CED of the biphasic reaction in batch mode (right) (scaled impact with respect to entry 1).

and to isolate the product, this interesting issue was addressed by means of hypothetical work-up steps considered in the environmental assessment. The theoretical work-up procedure for the isolation of the product and the adequate disposal of the ionic liquids mentioned above leads to significantly increased environmental impacts compared to the reactions without the consideration of a work-up procedure, as shown in Fig. 10. This result is mainly due to the evaporation of water from the aqueous phase prior to the disposal of the organic residues including the ionic liquids. In further experimental results, the aqueous phase will be substituted by an ionic liquid, being both a solvent and a phase transfer catalyst, to overcome the drawbacks of this laborious work-up procedure. By using the ionic liquid as a solvent, an automated phase separation and recycling of the ionic liquid may be possible.

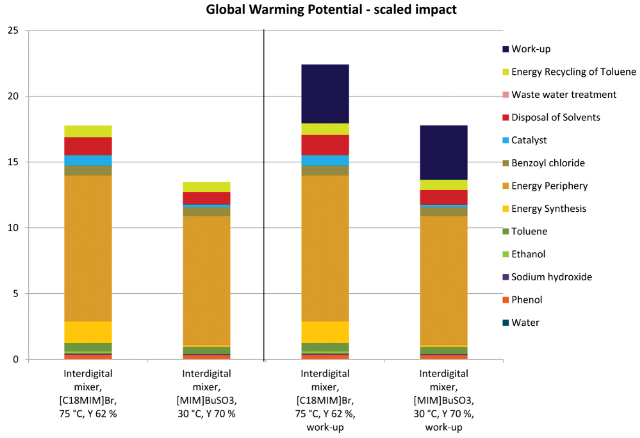


**Fig. 10** GWP for the continuously running esterification of phenol and benzoyl chloride under the implementation of [$C_{18}$MIM]Br and [MIM]$BuSO_3$ both without (left) and with (right) the consideration of a hypothetical work-up procedure.

In summary, the questions raised at the beginning of the process design can be answered as following:

*I. From an ecological point of view, the continuously running esterifications in an interdigital mixer under the implementation of ionic liquids are comparable to the reactions in batch mode at laboratory scale.*

*II. The energy demand of the plant periphery is the main influence on the environmental impacts of the continuously running syntheses. This leads to the conclusion that the batch reactions may be more environmentally benign because less energy is needed. However, this advantage becomes neutralized at industrial scale as pumps and controlling systems are needed for batch processes as well. Then, the continuously running processes should result in significantly lower environmental impacts.*

*III. The environmental burdens of the ionic liquids used as phase transfer catalysts are considerably smaller compared to the higher yields obtained by their usage. Thus, the higher yields obtained outweigh the environmental impacts of the supply of ionic liquids.*

*IV. Without the implementation of a catalyst, the herringbone structured mixer is more advantageous than the interdigital mixer. In the case of the implementation of [$C_{18}$MIM]Br, the interdigital mixer performs best, followed by the emulsification mixer and the herringbone structured mixer.*

*V. From an ecological point of view, [BMIM]Cl is the most beneficial ionic liquid used as phase transfer catalyst followed by [MIM]$BuSO_3$, since [$C_{18}$MIM]Br is synthesized under energy demanding conditions at 90 °C for 48 h.*

*VI. The work-up procedure considered increases the environmental burdens of the process considerably. Thus, this step is crucial in the SLCA to avoid problem shifts. Future work is focused on the substitution of the aqueous phase by a suitable ionic liquid allowing for an automated phase separation and recycling of the ionic liquid.*

## Economic evaluation

Similar or even better economic efficiencies are a premise for newly developed chemical processes to enter the market and compete with conventional processes. Thus, in addition to the SLCA investigations, cost analyses have been performed already at the laboratory scale to address the following issues:

*I. Is the biphasic esterification in microstructured reactors already economically competitive to the conventional production procedure of phenyl benzoate?*

*II. What kind of costs mainly affect the overall costs?*

*III. How will these main components be reduced by transferring the reaction to the production scale?*

The continuously running synthesis under implementation of [MIM]$BuSO_3$ was chosen for the cost assessment. This reaction resulted in the highest reaction yield and the lowest environmental impacts within their respective continuous processing modes.

The analysis, based on laboratory scale processing, was performed on a superficial level, considering the categories of fixed costs and variable costs of main cost items. The fixed costs were estimated by including plant purchase, maintenance and replacement of worn-out components. These costs were summed up over a time period of 10 years and divided by 10 to obtain the annual depreciation. Further, within the calculation of variable costs, the costs of materials and energy utilized in the reaction as well as in the hypothetically calculated work-up procedure were considered based on the experimental protocols and multiplied by actual catalogue prices.[50] In addition, the labour was estimated by multiplying the working time based on the reaction protocols with the hourly labour costs of a laboratory assistant. This included also the time which may be needed to work-up the reaction solution once per day. As a cautious estimate we considered a lower average gross wage of €18 per hour including also the employer's contribution to the social insurance.

These costs were summed up on an annual basis and related to the production capacity of phenyl benzoate to obtain the costs per kg of product. As the highest yield was obtained in the interdigital mixer by implementation of [MIM]$BuSO_3$ as phase transfer catalyst, this reaction was selected to discuss the cost analysis.

As was foreseeable at the laboratory scale, the total costs for producing 1 kg of phenyl benzoate by continuously running phase transfer catalysis in microstructured reactors under implementation of the ionic liquid have been found to be higher than the selling price of this substance. However, considering a batch process on the same laboratory scale (applying [BMIM]Cl as phase transfer catalyst) leads to a total cost 4.5 times higher due to very high labour costs. The total cost of the continuously running synthesis at the laboratory scale are composed of 43.8% fixed costs, 43.7% labour costs and 12.5% material costs. The material costs are mainly influenced by the hypothetical work-up procedure, the provision of toluene (although recycling of the solvent was assumed), the synthesis of [MIM]$BuSO_3$ at laboratory scale, the energy consumption of the microreactor plant as well as the provision of the reactants benzoyl chloride and phenol (Fig. 11).

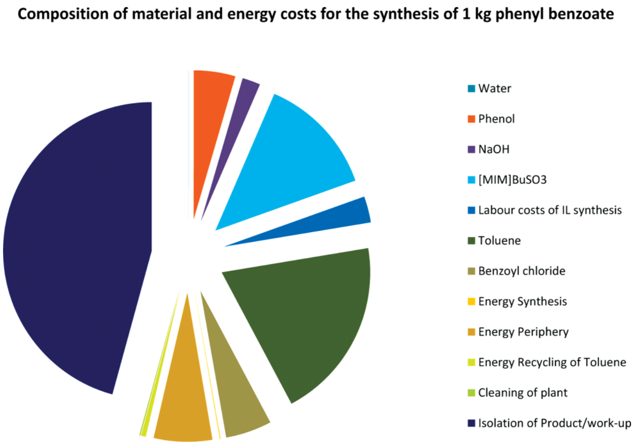


**Fig. 11** Variable costs (without labour costs of the esterification) for the continuously running synthesis of phenyl benzoate at laboratory scale.

A reduction in the total cost may be achieved by increasing the production capacity by a factor of at least 75 under the same reaction conditions (reaction temperature 30 °C, yield 70%, constant labour and fixed costs), which would be realizable in the lab scale plant. By this, the total costs can be decreased by 90% relative to the formerly discussed base case. The total costs consist of 5.5% fixed costs, 5.5% labour costs and 89% material costs (under consideration of lower unit costs for larger amounts of substances required for the synthesis). The higher production capacity assumed may be achieved by enhancing the flow rates under retention of yield and selectivity.

This calculation demonstrates that the compensation for the fixed and labour costs is feasible by higher production rates as the material becomes more influential. Usually, the share of the raw material costs is about 50 to 60% of the total costs.[51] Taking into account market prices for large purchase quantities of solvents and basic substances for the same set-up, an overall reduction in 99% of total costs seems to be possible for a future industrial scale processing.[43]

By estimating the costs for the continuously running synthesis under implementation of [MIM]$BuSO_3$ (entry 6) and comparison to the batch reaction under implementation of [BMIM]Cl as a phase transfer catalyst (entry 8) we found that:

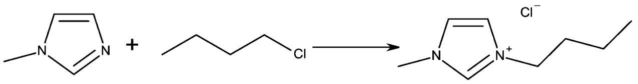
*I. The biphasic esterification carried out in the microstructured reactor at laboratory scale is more economically preferable than the batch reaction at laboratory scale.*

*II. The main cost drivers in the base case are fixed and labour costs, which may become negligible by enhancing the production capacities.*

*III. A reduction in 99% of total costs seems to be possible by transferring the continuously running biphasic esterification from laboratory scale to industrial scale.*

## Case study 2: synthesis of [BMIM]Cl

In the second case study, the environmental burdens and total costs of the synthesis of the ionic liquid [BMIM]Cl were investigated. This substance can be used, for example, as a phase transfer catalyst as was shown in case study 1. Although many ionic liquids are still under investigation, this is a very well-known representative of this class of substances. [BMIM]Cl was chosen as the second model substance for the comparative evaluation of batch and continuous processing, because in the solventless reaction (Scheme 3) of butyl chloride (BuCl) and 1-methylimidazole (MIM) a biphasic system is formed after the conversion of at least 8% 1-methylimidazole.[52] As this is also an exothermic reaction, it was regarded as being beneficially carried out in microstructured reactors.



**Scheme 3** Synthesis of the ionic liquid [BMIM]Cl from 1-methylimidazole and butyl chloride.

As a benchmark, two batch syntheses were investigated carried out at 80 °C[53] and 75 °C[52] by D. Kralisch and A. Große Böwing & A. Jess, respectively. Both batch reactions were conducted in a 500 mL round bottom flasks equipped with a reflux condenser and a mechanical stirrer. These results were compared to four continuously running synthesis scenarios at temperatures of 145 °C and 150 °C under the employment of a Knauer Smartmix™ mixer, which were conducted by Loewe and co-workers.[46] All reaction conditions considered are summarized in Table 2.

The reaction mixtures were heated up by oil bath heating in all cases. Contrary to case study 1, the estimation of the energy

**Table 2** Reaction conditions used for SLCA investigation of the biphasic reaction of butyl chloride and 1-methylimidazole giving [BMIM]Cl[46,52,53]

| Entry | Processing mode | Molar ratio (BuCl : MIM) | $T/°C$ | Residence time [min] | Yield [%] |
|---|---|---|---|---|---|
| 1 | Batch | 1.2 | 75 | 2820 (47 h) | 96 |
| 2 | Batch | 1.4 | 80 | 1305 (21.75 h) | 70 |
| 3 | Continuous | 1.2 | 145 | 31.7 | 87 |
| 4 | Continuous | 2 | 145 | 23.4 | 70 |
| 5 | Continuous | 2 | 150 | 12.3 | 77 |
| 6 | Continuous | 1 | 150 | 12.1 | 82 |

needed during the syntheses by means of thermodynamic data was not suitable, since this is a highly exothermic reaction. Thus, the energy consumption of the oil bath heating was estimated based on energy measurements. This can be regarded as a conservative approach because thermal effects of the synthesis were mainly neglected. Furthermore, in the case of the continuously running reactions the energy of the periphery (pumps, controlling instruments) were estimated based on the data investigated in case study 1. Here, we assumed that the same microreaction plant could be used for the synthesis of the ionic liquid, too.

Two different work-up procedures were considered depending on the processing mode: in the batch syntheses, a dilution in water and extraction with methyl *tert*-butyl ether was assumed as described by Kralisch.[53] Afterwards, the ether extracts were collected and the ether was distilled off with a recovery rate of 90%. In case of the continuously running synthesis, the residual butyl chloride was distilled off and the crude product was recrystallized from acetone.[46]

## Results

As the functional unit, 1 kg [BMIM]Cl was chosen to investigate the environmental burdens as well as the total costs of this biphasic reaction.

### Simplified life cycle assessment

The reactions were carried out under varying reaction conditions in two different processing modes (see Table 2). Thus, by means of SLCA the following aspects were investigated:

*I. Which reaction component shows the main influence on the environmental impacts?*

*II. Which molar ratio of both reactants is the most environmentally benign?*

*III. Do the reaction temperature and the residence time influence the environmental performance of the system under investigation?*

*IV. How does the applied work-up procedure affect the environmental burdens of the reaction?*

*V. Which processing mode is more beneficial from an ecological point of view?*

In Fig. 12, an overview of the environmental impacts of the reactions investigated is given. As the results obtained by Große Böwing and Jess were considered as a reference, entry 1 was chosen to scale the environmental impacts. It can be seen that processes with a reaction yield lower than 80% (entries 2, 4, 5) are less environmentally benign than the reference synthesis.

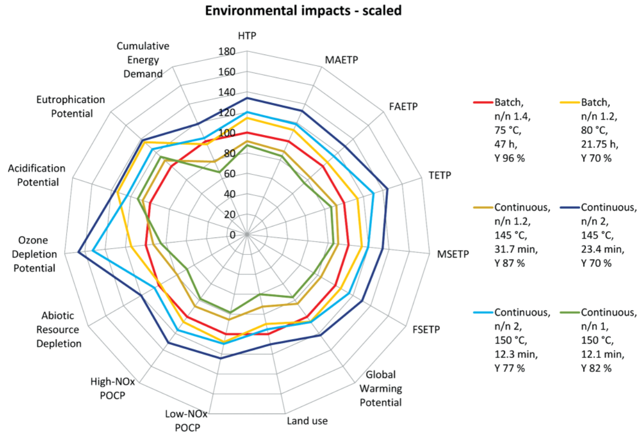


**Fig. 12** Overview of environmental impacts of the synthesis of [BMIM]Cl without solvent.

This outcome is independent, whether the reaction is carried out as a batch reaction or as a continuously running reaction.

The environmental impacts, *e.g.* the HTP (Fig. 13), of the syntheses are dominated by the provision of the reactants 1-methylimidazole and butyl chloride. Thus, the molar ratio of both substances is of great importance for the environmental performance of the reaction. Because of this, the continuously running reactions with a molar ratio BuCl : MIM of 1.2 : 1 and 1 : 1 (entries 3 and 4) resulted in the lowest environmental impacts.

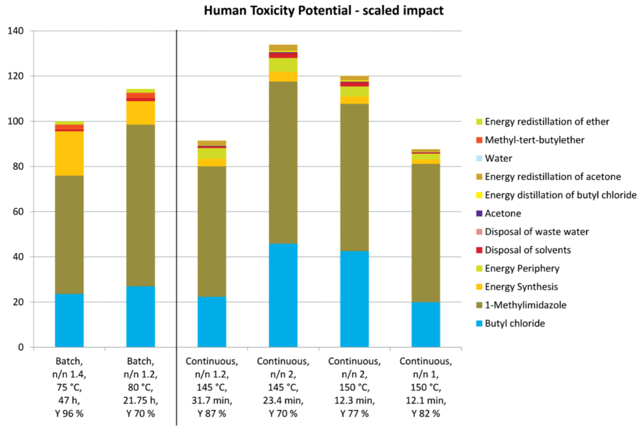


**Fig. 13** HTP of the synthesis of [BMIM]Cl from butyl chloride and 1-methylimidazole without solvent in batch (left) and continuously (right) running reactions.

In addition, the energy consumed during the synthesis strongly influences the overall GWP of the reaction procedures

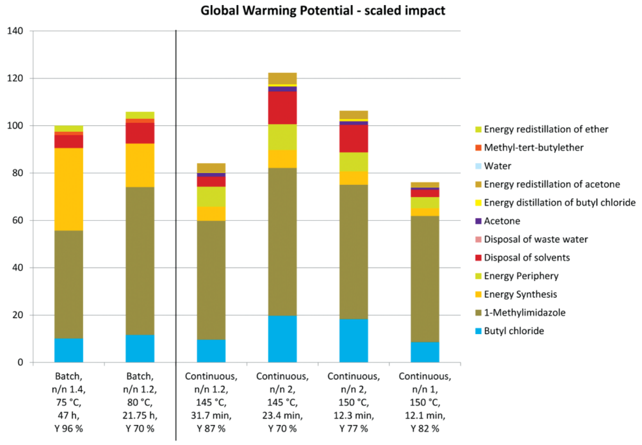


**Fig. 14** GWP of the synthesis of [BMIM]Cl from butyl chloride and 1-methylimidazole without solvent in batch (left) and continuously (right) running reactions.

considered (Fig. 14). In consequence, higher GWPs have been found for the syntheses under batch conditions compared to the continuously running reactions at 145 °C and 150 °C with molar ratios BuCl : MIM of 1.2 : 1 and 1 : 1 (entries 3 and 5). In microstructured reactors, the synthesis can be performed at higher temperatures to activate the reaction. Due to the high surface-to-volume ratio of the microreactor, the generated heat can be removed more efficiently to avoid a thermal runaway. Thus, the residence times can be shortened to several minutes instead of a couple of hours. Clear ecological advantages for the continuously running syntheses in a microreaction set-up can be gained from that, as shown in the examples of HTP and GWP in Fig. 13 and 14.

The share of the respective work-up procedures are comparably low in all cases and more or less independent from the work-up procedure assumed. The HTP (Fig. 13) of the respective procedures are 3.5% in the case of the batch syntheses and 1.7 to 2.8% of the overall environmental impact depending on the reaction yield obtained during the continuously running syntheses. In the GWP (Fig. 14), the share of the work-up procedure in the overall environmental burden is 4 to 4.5% for the batch syntheses and 4 to 6.7% for the continuously running reactions. These results are basically caused by the provision of the organic solvent for extraction or recrystallization and the energy consumed by distillation of the solvent. The reuse of the organic solvents is already included in this estimation. These simple procedures for product isolation can be applied because of the solventless reaction.

The questions raised at the beginning of the the SLCA investigations could be answered as follows:

*I. Both reactants, 1-methylimidazole and butyl chloride, considerably influence the environmental impacts of the syntheses under investigation. Furthermore, the energy consumed during the reaction may also have a strong influence on the environmental burdens.*

*II. The molar ratio of both reactants should be kept as low as possible. The ideal ratio is 1 : 1. Thus, a continuously running synthesis at 150 °C employing equal amounts of reactants has been found to be the most environmentally benign synthesis pathway considered in this investigation.*

*III. Reaction temperatures and residence times influence the environmental burdens of the process only indirectly. Due to the exothermic character of this process, high reaction temperatures can only be handled safely in continuously running reactors with short residence times.*

*IV. The work-up procedures considered have only a minor influence on environmental burdens (<10%).*

*V. From an ecological point of view, the continuously running processes are more environmentally benign than the ionic liquid syntheses in batch mode. This result is only valid if high reaction yields can be obtained, low molar ratios are applied and short residence times can be realized.*

## Economic evaluation

In addition to the SLCA investigations, a rough cost estimation was applied to the solventless synthesis of [BMIM]Cl in laboratory scale. By this, the following questions were examined:

*I. What kind of costs mainly influence the total costs?*

*II. Which processing mode should be preferred from an economic point of view?*

*III. Which reaction component has the main influence on the variable costs?*

According to a lack of more detailed information, the fixed costs for the continuously operating microreaction plant as well as labour costs were estimated based on the information gathered in case study 1. This was assumed to be an appropriate approach, since the microreaction plant was specifically designed for biphasic reactions.

In Fig. 15, the total costs of the syntheses of [BMIM]Cl in laboratory scale are presented, scaled to the estimation of total costs of the batch synthesis published by Große Böwing and Jess.[52] Due to the high labour costs, the total costs of the batch syntheses are considerably higher than the total costs of the syntheses performed in a fully automated microreaction plant. In the case of the continuously running syntheses, labour costs and variable cost have about equal shares in the total costs.

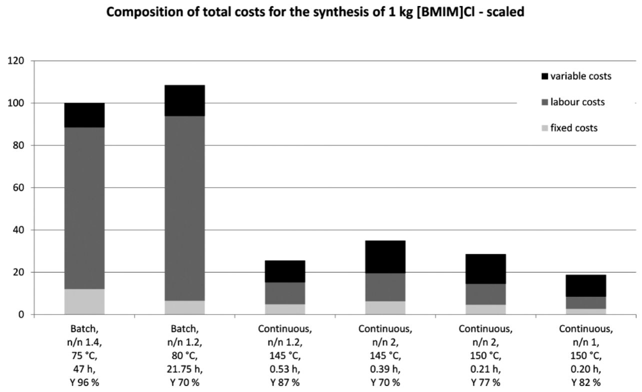


**Fig. 15** Composition of total costs of the synthesis of [BMIM]Cl from butyl chloride and 1-methylimidazole without solvent in batch (left) and continuously running (right) reactions.

The lowest total costs are caused by the continuously running synthesis at 150 °C with a molar ratio BuCl:MIM of 1 : 1, resulting in a reaction yield of 82%. According to Fig. 16, the variable costs of this synthesis mainly consist of the purchase costs for the reactants, 1-methylimidazole and butyl chloride.

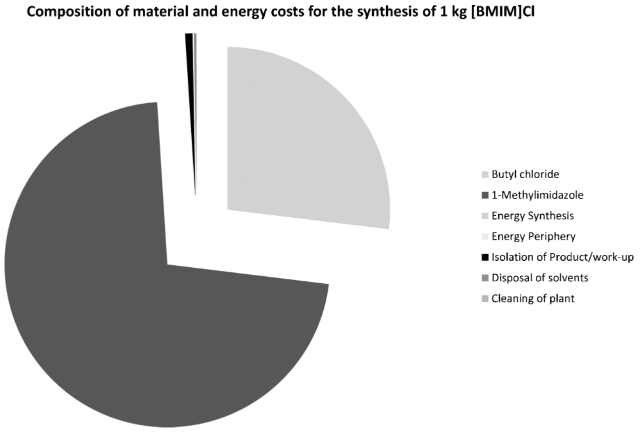


**Fig. 16** Composition of variable costs of the synthesis of [BMIM]Cl from butyl chloride and 1-methylimidazole without solvent.

From the comparison of batch and continuously running syntheses in laboratory scale it was concluded, that:

*I. The total costs of the batch syntheses consist mainly of labour costs, whereas the total costs of the continuous reactions are equally dominated by labour and variable costs. Fixed costs have only a minor effect on the total costs in both processing modes.*

*II. As the continuous reactions in a fully automated microreaction plant lead to considerably lower total costs compared to batch reactions, this processing mode should be preferred from an economic point of view for further process design studies.*

*III. The variable costs are mainly influenced by the provision of reactants.*

## Conclusions

We have presented our research accompanying SLCA complemented by a superficial cost analysis which is illustrated by discussing the two case studies: continuously running phase transfer catalysis of benzoyl chloride and phenol giving phenyl benzoate, and the solventless synthesis of the ionic liquid [BMIM]Cl. Both reactions are multiphase processes which can be carried out beneficially in microstructured reactors.

The environmental burdens of the synthesis of phenyl benzoate were essentially influenced by the reaction yields obtained, as higher yields lead to less process waste and to a more efficient use of resources. Thus, the energy consumed by the fully automated microreactor plant exhibited the highest contribution to the Global Warming Potential, whereas the Human Toxicity Potential was almost equally dominated by the energy consumption and the provision of phenol. The performance of different micromixing structures has been found to be dependent on other process parameters, *e.g.*, the utilization of a phase transfer catalyst. In comparison, the interdigital micromixer (IMM) in combination with [MIM]BuSO$_3$ and a reaction temperature of 30 °C have shown the lowest environmental impact of all continuously running synthesis alternatives.

As this process is still under development, there a hypothetical work-up procedure was considered. Future experimental work will focus on the continuously operated phase separation leading to a simplified product isolation by distillation from the organic phase as well as a recovery of the ionic liquid for further processing.

In the case of the synthesis of the ionic liquid [BMIM]Cl, the environmental burdens were influenced by both the reaction yields obtained and the molar ratio of the reactants 1-methylimidazole and butyl chloride. Thus, the most environmentally benign synthesis was carried out in the continuously operated microreaction plant at 150 °C and equal amounts of reactants.

Work-up procedures were considered for both processing modes. In case study 2, the reaction was conducted without an additional solvent. Thus, the removal of a solvent prior to product isolation was not necessary. This led to simplified work-up procedures compared to other reaction types implementing organic solvents, *e.g.*, case study 1. By this, the product isolation had a minor influence on the environmental burdens of the reactions under investigation.

Additionally, the economic potential of both processes was demonstrated although at a screening level. The superficial cost estimation at laboratory scale of the synthesis of phenyl benzoate showed that, under laboratory scale conditions, the batch syntheses result in higher costs due to higher manpower requirements. Under industrial scale conditions, syntheses with the highest yields will be the most cost efficient, since the total costs will be influenced mainly by the costs of raw materials. Fixed costs, especially investment costs, will have a minor share.

In conclusion, helpful decision support could be gained from these evaluations, paving the way for a deliberately green process design.

## Experimental

The phase transfer catalytic reactions were carried out under standardized two-phase conditions. The inorganic (aqueous) phase contained 0.3 mol L$^{-1}$ phenol, 0.35 mol L$^{-1}$ sodium hydroxide and 0.01 mol L$^{-1}$ of the selected phase transfer catalyst while the organic phase (toluene) contained 0.1 mol L$^{-1}$ benzoyl chloride. With the applied volume flows of 0.3 mL min$^{-1}$ of the inorganic phase (0.09 mol min$^{-1}$ phenol) and 0.9 mL min$^{-1}$ of the organic phase (0.09 mol min$^{-1}$ benzoyl chloride) dispersions were formed in the micromixers chosen. To calculate kinetic data, experiments were performed in a thermostatted water bath at different temperatures ranging from 20 °C to 80 °C. It was assumed that the temperature inside the glass microreactors is equal to the outside thermostatted fluid due to their very small inner volumes.

The concentrations of phenyl benzoate, benzoyl chloride and benzoic acid were determined by a Thermo Nicolet 380 FT-IR spectrometer equipped with a Smart MIR Fibre Port (Themo), connected to a DiProbe-ATR infrared fibre sensor (ifs Aachen, Germany). OMNIC 7.3 software was used for data acquisition and subsequently analysed by TQ Analyst version 6.2.1.509. As a calibration model for determining phenyl benzoate, benzoyl chloride and benzoic acid in toluene, a PLS algorithm (partial least squares) was applied with the assumption that concentrations of each component below 0.1 mol L$^{-1}$ does not influence the concentration of toluene significantly.

## Abbreviations

| | |
|---|---|
| [BMIM]Cl | 1-Butyl-3-methylimidazolium chloride |
| [C$_{18}$MIM]Br | 1-Octadecyl-3-methylimidazolium bromide |
| [MIM]BuSO$_3$ | 1-Butylsulfonate-3-methylimidazolium |
| BuCl | Butyl chloride |
| CED | Cumulative Energy Demand |
| CML | Institute of Environmental Science, Universiteit Leiden, The Netherlands |
| EATOS | Environmental Assessment Tool for Organic Syntheses |
| ECO | Ecological and Economic Optimisation |
| E-Factor | Environmental factor |
| EHS | Environmental Health and Safety |
| ELI | Energy Loss Index |
| FAETP | Fresh Water Aquatic Ecotoxicity Potential |
| FSETP | Fresh Water Sedimental Ecotoxicity Potential |
| GWP | Global Warming Potential |
| HTP | Human Toxicity Potential |
| IMM | Institut fuer Mikrotechnik Mainz |
| ISO | International Standard Organisation |
| LCA | Life Cycle Assessment |
| LCI | Life Cycle Inventory |
| LCIA | Life Cycle Impact Assessment |
| MAETP | Marine Aquatic Ecotoxicity Potential |
| MSETP | Marine Sedimental Ecotoxicity Potential |
| MIM | 1-Methylimidazole |
| MIPS | Material intensity per service unit |
| PTC | Phase transfer catalysis |
| POCP | Photochemical Ozone Creation Potential |
| R&D | Research and Development |
| SETAC | Society of Environmental Chemistry and Toxicology |
| SLCA | Simplified Life Cycle Assessment |
| TETP | Terrestrial Ecotoxicity Potential |
| TAPPS | Total annualized profit per service unit |

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