Life Cycle Analysis: Assessment of Technologies for Droplet Separation – A Case Study

Mandy Paschetag[1,*], André Paschetag[1], Florian Merkel[2], Christian Mehringer[3], and Stephan Scholl[1]

DOI: 10.1002/cite.202000255

For the assessment of separation technologies from an ecological and economic perspective, a case study was performed to investigate the influence of entrainment on energy and resource demand of a single apparatus and on a single production process. Taking the example of the Rectisol process, the influence of droplet entrainment on individual separation equipment as well as on the process as a whole was identified via flowsheet simulation. Based on the calculated mass and energy balances, an LCA and LCC approach was used for the quantification of the entrainment influence.

Keywords: Chemical industry, Energy and resource efficiency, Life cycle assessment, Life cycle costing, Process design

Received: December 09, 2020; *revised:* April 02, 2021; *accepted:* April 07, 2021

1 Introduction

Through commencement of the Climate Change Act, the German industrial sector set the goal to reduce their greenhouse gas emissions by up to 25 % until 2030 following the maximum permitted values of 186 million tons of emitted CO_2 equivalents in 2020 [1]. This represents a major challenge and forces emitters to deal intensively with the issues of energy and resource efficiency. For this very reason, many companies voluntarily participate in associations such as SPIRE [2], which aim to strengthen the European industry by process improvements as well as reduction of energy and resource consumption and waste volumes. The combined goal is a decrease of energy consumption in the process industry by 30 % and the primary, non-renewable raw material intensity by 20 %. As a superordinate result, the reduction of the carbon footprint by 40 % by 2030 compared to the period 2008 ... 2011 is targeted. [3]

The chemical industry is one of the most energy- and emission-intensive sectors in Germany, on the one hand due to high energy and heat requirements and the associated need for fossil raw materials and on the other hand due to the reactants and auxiliary materials likewise based on fossil raw materials such as natural gas and crude oil [4]. Fluid separation processes are some of the central unit operations in the material conversion industry. Vapor/liquid separation operations are usually the most energy-intensive process steps, due to the fact that evaporation and condensation processes are usually performed subsequently several times. In such processes the desired mass transfer can be promoted through enlargement of the specific interfacial area. A larger phase interface can be achieved through decreased drop or bubble diameters. Subsequently, the two phases must be coalesced again and separated – ideally without carry-over of one phase into the other. The entrainment of droplets in the vapor phase or vapor bubbles in the liquid phase partially nullifies the invested separation expenditures and thus reduces the energy efficiency of the separation. This carry-over may also result in corrosion and/or safety related issues on downstream process areas following the separation, which are often not designed for the entrained fluids.

The joint research project "Droplet formation and reduction in mass transfer apparatus – TERESA" aims to provide improved design methods for phase separation apparatuses and droplet separation internals. The further development and improvement of the design basis for the prevention of entrainment in the column head and sump as well as in the feed line combined with the feed inlet serve to improve the ecological and economic performance of material conversion processes.

Questions that need to be answered with regard to new technologies and their operation in the production process

[1]Mandy Paschetag, André Paschetag, Prof. Dr.-Ing. Stephan Scholl
m.paschetag@tu-braunschweig.de
Technische Universität Braunschweig, Institute for Chemical and Thermal Process Engineering, Langer Kamp 7, 38106 Braunschweig, Germany.

[2]Dr. Florian Merkel
weyer gruppe, horst weyer und partner GmbH, Schillingsstrasse 329, 52355 Düren, Germany.

[3]Dr. Christian Mehringer
RVT Process Equipment GmbH, Paul-Rauschert-Strasse 6, 96349 Steinwiesen, Germany.

include "What influence does the newly developed technology have on the functional performance of a process itself as well as on the environmental and cost performance?" and "Are energy and CO_2 saving potentials available and if so, in which quantity?".

In this paper, the use of a droplet separator and its effects on the performance as well as the potential environmental impact of a production process in the chemical industry are presented. Based on a case study, a defined throughput of a production process is used to compare separation columns, which operate with and without a droplet separator. In addition to the ecological assessment, an economic consideration is performed. The ecological assessment follows the method of life cycle assessment (LCA) with a cradle-to-gate approach while the method of life cycle costing (LCC) is utilized to quantify the economic effects from the operator's point of view.

2 Assessment of New Technologies

For the holistic assessment of a new technology, a consideration over the whole life cycle is necessary, on the one hand to identify hot spots of ecological or economic impacts and on the other to track a shifting of potential impacts between life cycle phases. For example, an additional apparatus can be advantageous in operation but due to its structural characteristics and the use of special materials in its manufacturing and disposal, the addition can involve high expenditures. In general, two factors have to be considered for the assessment of a new equipment technology. These are the expenditures directly related to the apparatus and the resulting influence on the overall impact of a process through the application of such technology.

The assessment of new technologies in an early stage of process development can support the design choices by highlighting the corresponding implications on the environmental and economic performance. To investigate the possible future performance, scenarios can be defined to explore, amongst others, the influence resulting from the surrounding production infrastructure, e.g., [5–8]. The inclusion of such information can reduce operating costs and avoid unnecessary environmental burdens or investment.

Unfortunately, an incomplete data base in the early stage of process development as well as unknown scale up effects [9] and a high uncertainty do not allow a reliable statement like an ex-post LCA study based on a well-defined system would do [10]. Parvatker and Eckelmann [11] present a hierarchy of methods to address the scarcity and data/time requirements of life cycle inventory data. Data collected directly from the production plant or LCI-databases are classified with the lowest level of uncertainty and the highest level of requirements and accuracy; within the next rank the process simulation tools are listed. Simulation tools like Aspen plus, ChEMCAD, or ProSim are commonly used tools in the engineering workflow in the process industries and often used during the design phases to model the industrial scale of an investigated production process or single unit operations. Based on thermodynamic models and material properties the consumption data can be estimated and aggregated to prepare an LCI. Approaches to otherwise consider the influence of upscaling effects in LCA are shown, e.g., in [12–14].

The life cycle of an apparatus in a chemical production plant can be represented by the phases *resource extraction, material refinement, apparatus engineering*, *construction, production operation, dismantling,* and *recycling/disposal* [15]. The *resource extraction* contains the supply of ores, rubber, carbon, etc. as well as the extraction of fossil and renewable energy sources and their transformation. The subsequent life cycle phase *material refinement* describes the processing of the raw materials and the production of the required materials for manufacturing (e.g., pig iron extraction, steel production or forming). *Apparatus engineering* includes the processing of steel products into apparatuses by various manufacturing processes, such as forming, joining or coating and changes in material properties, e.g., sintering. The stage of *construction* applied to the life cycle of an individual piece of equipment includes the expenditure required to install the equipment in existing or to be constructed plant structures and the associated expenditures for piping, installation or conversion of the I&C technology and integration into existing operating supply networks. The phase *production operation* includes the expenditures over the operating time, mainly the maintenance as well as the energy and materials caused by the operation of production processes as well as the expenditures due to the operational infrastructure. The life cycle phase *recycling/disposal*, which follows the production phase and the dismantling of the plant, describes the recovery and disposal paths of the materials used in the production plant.

According to the EU guideline for the calculation of the environmental footprint of products (product environmental footprint, PEF), the cut-off of ecological expenditure is not permitted while a linear depreciation of capital goods (e.g., apparatuses) over the use phase is prescribed [16]. Due to the complexity of the associated value chains of the capital goods, the depreciation fails primarily due to the necessary level of detail as shown by Hausschild [17].

Especially the ecological assessment is associated with challenges in data acquisition when considering the life cycle: The diversity of materials in a production plant and the level of detail required to record expenses, e.g., those associated with individual production steps in the manufacture of equipment, result in a considerable effort when collecting data. With regard to the production plant, the apparatus and equipment are usually purchased from different manufacturers. Among other things, location-specific aspects play a role here due to the production sites from all over the world. Databases such as ecoinvent support the estimation of expenditures with generic datasets. However, specific records for the production of different types of equipment (e.g., heat exchangers, separation columns, reactors) do as of yet not exist. Hischier et al. [18] refer to a generally valid data set ("chemical factory, organics"), which is available in the ecoinvent database. This can serve as a guide for a first estimation without taking into account the variability of the production facilities [19]. However, such a data set is unsuitable for the evaluation of new equipment technologies as well as the evaluation of different scenarios regarding the production context. In case of missing data the ILCD-Handbook recommends an estimation of the materials and their masses used in order to illustrate the influence of the equipment [20].

Expenditures related to the production plant are often regarded as negligible and cut off in the assessment rationalized by the small impact in relation the total ecological expenditures [21–26]. In this context, the studies of different authors, which take the plant equipment into account, show diverging results. For example, Griffiths et al. [27] compare different iron and palladium-based catalysts in nanoparticle format based on laboratory data including the impact of the laboratory plant. However, due to an electrically heated synthesis with high temperature sections and the complex metal catalysts, all other inputs or outputs play a minor role. Other authors [5, 28, 29] also conducted studies on the assessment of new technologies under consideration of apparatuses or production plants by taking up the approach described in the ILCD-Handbook in regards to the estimation of materials/masses [20] and quantify a significant proportion in various environmental impact categories.

The examples given above for the assessment of new technologies result in diverging statements on the apparatus influence and highlight that data gaps for individual life cycle phases and the limited consideration of these phases do not allow a generally valid statement regarding the influence on the ecological performance of individual production processes. For the consideration of the influence caused by additional installations in an apparatus, the approach of the ILCD-Handbook [20] as well as by Wesche et al. [30] will be used within the present investigation. Of the apparatus, its manufacturing materials as well as their related expenditures are assessed, whereas the influence resulting from the implementation of a new technology on the production process is determined via flow sheet simulation (FSS) to ensure a high level of data accuracy.

3 Simulation of Entrainment

3.1 Simulation of Entrainment in a Single Separation Column

Using a model of a C_nH_m separation column, the influence of entrainment on the performance of an individual apparatus is simulated and quantified. The column is simulated as an independent combination of equilibrium stages with a manual adjustment possibility of the entrainment (Fig. 1a).

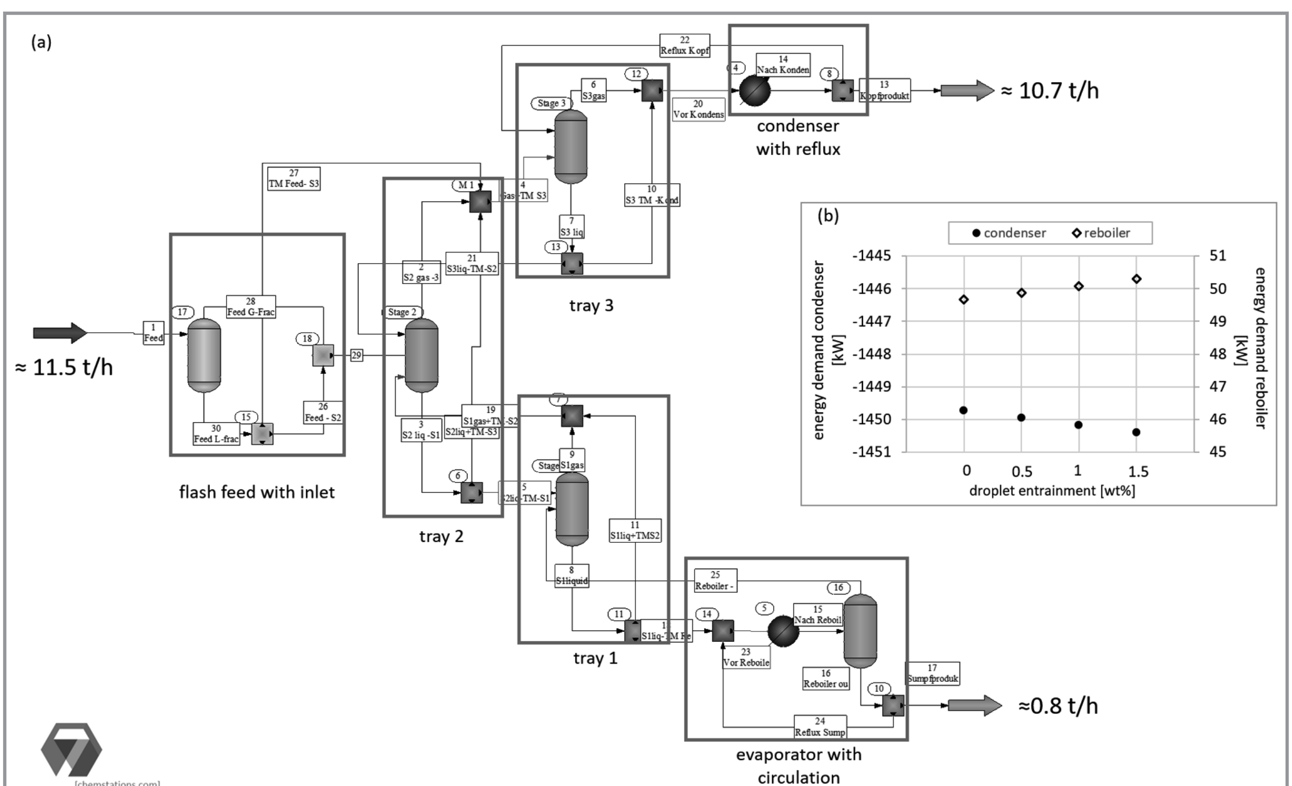

Figure 1. Detailed flow sheet simulation model of a C_nH_m separation column (a); energy demand of reboiler and condenser as a function of entrainment (b).

The model tracks the composition of the gas and liquid phase for each tray. The individual trays of the column are each implemented as an individual flash (stage 1–3). To simulate entrainment, each tray is followed by a mixer and divider. For the third tray (stage 3) these are, e.g., unit op (13) and (14). The divider separates an individually specified amount of fluid from the liquid phase and feeds it into the mixer in the gaseous outlet stream of the tray. This way, the gas phase emerging from the tray of interest can be manually loaded with an additional liquid quantity of entrainment. The simulation of the entrainment can therefore be carried out in high detail and the influence on the product quality can be quantified. By simulating a condenser (4) with a subsequent divider (8) the reflux ratio can be precisely adjusted to negate effects on product quality. The liquid phase from tray 1 (stage 1) flows into an evaporator with circulation. The influence of the entrainment on the energy demand of the column can be determined by means of monitoring the energy consumption of condenser and evaporator.

For the investigations, a two-component mixture with a satisfactory boiling point difference and a low boiler content of 93 wt % is considered. The mixture enters the column with a gas content of 0.996 wt/wt. The total mass flow in the feed amounts to 11.5 $t\,h^{-1}$. Fig. 1b shows the changes in the energy requirements of condenser and evaporator in a sensitivity study. The effects of entrainment at 0, 0.5, 1, and 1.5 wt % across all trays and the feed inlet are investigated. The specification of the product flow at the head is set at 0.99589 wt % low boiler content. The reflux ratio for the investigated entrainments to achieve the required specification vary in the corridor of 0.2000 ... 0.2079. The deviations of the specific energy input for 0 and 1.5 % entrainment are 0.43 $kJ\,kg_{spec.product}^{-1}$. In total, this leads to an additional thermal energy demand of approx. 37 GJ per production year.

3.2 Simulation of Entrainment in a Production Process

The scope of the investigations is extended to quantify the influence of a new technology in a production process. For this purpose, a process for the purification of synthesis gas is also modelled in a flow sheet simulation (Fig. 2). The simulation depicts the Rectisol process and is based on the requirements and specifications as shown in [31], supported by additional information from [32].

The Rectisol process represents a typical process in the petrochemical industry and is used to separate acidic components from synthesis gas using methanol as scrubbing agent. The process can be divided into three main process tasks: (I) Absorption of hydrogen sulfide (H_2S) and carbon dioxide (CO_2), (II) carbon monoxide (CO) and hydrogen (H_2) recovery, and (III) desorption of CO_2 and thus recovery of the washing agent circulating in the process (circulation not shown in simulation).

To determine the effects of entrainment in an apparatus in the context of an entire production process, the entrainment is simulated at the head of column K1 similar to the procedure in the C_nH_m separation column. Similar to the simulation of the C_nH_m separation column, a sensitivity study is performed in which the entrainment is varied between 0, 0.5, 1, and 1.5 wt %. The results of the analysis are shown in Tab. 1.

Even in the case of 0 wt % entrainment, a make-up stream of 60 $kg\,h^{-1}$ is required to compensate losses via the gas phase.

With rising entrainment, the data show a significant increase in virgin washing agent (methanol) demand from 60 $kg\,h^{-1}$ (0 wt %) to 11 309 $kg\,h^{-1}$ (1.5 wt %), which must be replaced in the process. The demand for thermal and electrical energy, however, decreases slightly with increasing entrainment. This is due to the fact that the entrainment of

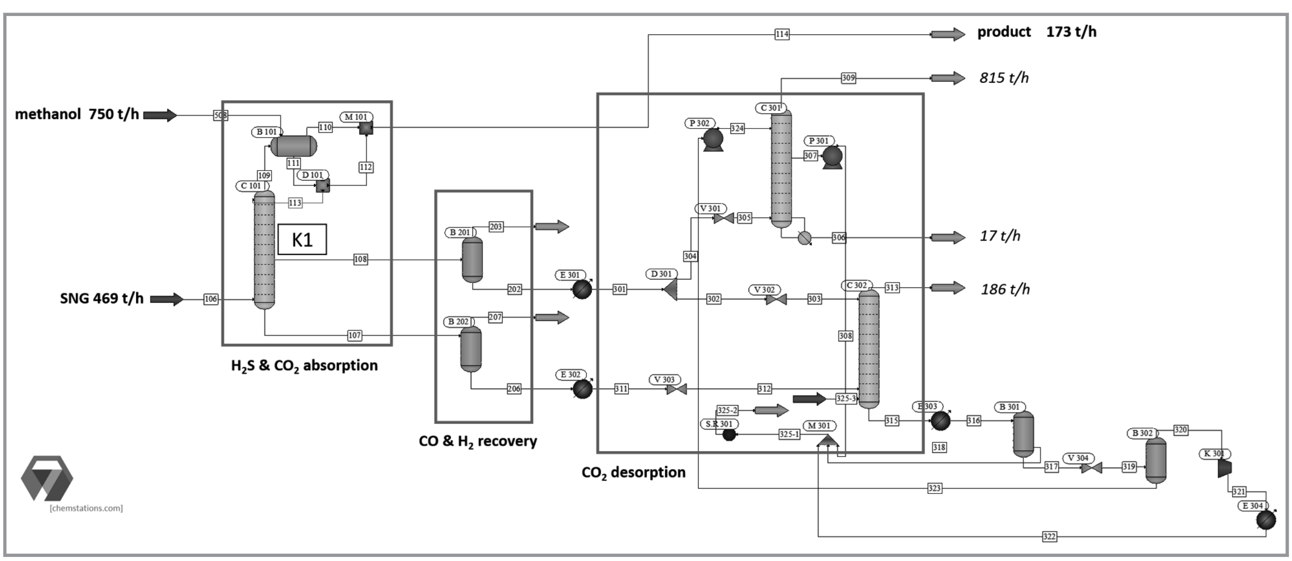

Figure 2. Flow sheet model of the Rectisol process modeled with CHEMCAD [33].

Table 1. Balance of the Rectisol process for different percentages (wt %) of entrainment.

Material/energy		Unit	0 wt %	0.5 wt %	1 wt %	1.5 wt %
INPUT						
Raw gas		kg h^{-1}	468 820	468 820	468 820	468 820
Methanol		kg h^{-1}	60	3810	7559	11 309
Thermal energy	Heating	kW	9412	9419	9428	9435
	Cooling	kW	–12 170	–12 165	–12 158	–12 153
	Evaporation	kW	288 278	286 833	285 389	283 972
Electrical energy		kWh	1077	1072	1067	1062
Sum mass flow		kg h^{-1}	468 880	472 630	476 379	480 129
Sum energy		kW	309 860	308 418	306 975	305 560
		kWh	1077	1072	1067	1062
OUTPUT						
By-products		kg h^{-1}	295 534	294 328	293 106	291 876
Synthesis gas		kg h^{-1}	173 441	178 405	183 366	188 355
	MeOH	*kg h^{-1}*	*60*	*3810*	*7559*	*11 309*
	CO_2	*kg h^{-1}*	*27 465*	*28 647*	*29 827*	*31 033*
	H_2S	*kg h^{-1}*	*0*	*0*	*0*	*0*
	CO	*kg h^{-1}*	*125 228*	*125 258*	*125 288*	*125 319*
	N_2	*kg h^{-1}*	*2 232*	*2232*	*2232*	*2232*
	H_2	*kg h^{-1}*	*18 457*	*18 458*	*18 460*	*18 461*
Exhaust heat		kW	207	206	205	204
Sum mass flow		kg h^{-1}	468 976	472 732	476 472	480 231
Sum energy		kW	207	206	205	204

the methanol reduces the material flows in the subsequent purification steps. Among other things, the material flow leaving column K1 in the sump contains less methanol, which would otherwise have been separated and recycled in the downstream process stages.

The composition of the product stream leaving the absorber (column K1) (<114>) is shown in the balance sheet (in italics). In addition to the entrained amount of methanol, the amount of the impurity carbon dioxide also increases by 3586 kg h^{-1}. The reason is the absorption of carbon dioxide in the washing agent and, in the case of entrainment, the discharge from the column overhead. The resulting additional impurities in the product stream have to be separated in supplementary purification steps. This results in further expenditures in terms of equipment and energy if the washing agent needs to be recovered.

In the following case study, an additional purification is integrated into the investigations in order to assess the effects of entrainment in the production process from both an ecological and economic point of view. To calculate the mass and energy balances for the LCI the flow sheet simulation is used (Fig. 2).

4 Case Study

A case study for the Rectisol process has been set up to assess the ecological and economic impact of entrainment. A scenario with (see Sect. 3) and without entrainment as well as the resulting effects on the whole process are compared.

4.1 Description of the Case Study

4.1.1 Current State

As a basis for the comparison an entrainment of 1.5 of the liquid phase is assumed in the current state. For the assessment, the balance shown in Tab. 1 is extended to account for the additional expenditures for the entrained solvent methanol. The influence of the additional expenditures is estimated through an added purification step, which includes three heat exchangers (HEX), an expander, a pump and a flash vessel, inserted into stream <114>, cf. Fig. 2, as well as a recycling stream. The extended downstream processing reduces the solvent loss of methanol by approx. 68 % from 11 309 $t\,h^{-1}$ (see Tab. 1) to 3637 $t\,h^{-1}$, whereas 7672 $t\,h^{-1}$ are fed back. The operation of these additional equipment increases the energy demand provided through utilities by 15 905 kW. The assessment of the current state also considers the additional material quantities of stainless steel in the ecological assessment as well as the additional investments and the revenues from disposal in the economic assessment.

4.1.2 With Droplet Separator

For this case a liquid phase entrainment of 0 wt % is assumed. In the column K1 a droplet separator is located to prevent the entrainment of methanol. In the assessment a solvent loss of approx. 60 $t\,h^{-1}$ is taken into account entrained by gas phase based on the vapor-liquid equilibrium. Short-cut sizing of the column results in a diameter of 4.0 m at a material thickness of 16 mm. The calculated weight of the necessary stainless-steel separator is 700 kg. The pressure loss resulting from the installation is, in the opinion of interviewed experts low, but is nevertheless taken into account for comparative purposes. The energy expenditure associated with the pressure loss is assumed by the experts to be 112 500 $kWh\,a^{-1}$. No further consumption is attributed to the usage of the droplet separator.

4.2 Scope of Investigation

For the assessment the differences between the described cases over the life cycle are analyzed. In the following, the considered life cycle phases and the assumptions made in the comparative studies are presented as well as the material and energy flows which are taken into account.

4.2.1 Ecological Assessment

For the assessment of the ecological expenditures the life cycle of the plant as well as the process as part of a product life cycle are linked, whereby the consideration of the process is carried out by a cradle-to-gate approach. The investigation aims at the depiction of the influence of a droplet separator on the energy and resource demand as an example for the influence of equipment design. Furthermore, the expenditures caused by the provision, maintenance and disposal of said equipment has to be quantified.

Fig. 3 shows the life cycle phases of an equipment as described in detail in Sect. 2. In the study, the corresponding expenditures resulting from the additional purification step (current state) or the droplet separator are taken into account. The life cycle phases colored in white are not included in the analysis due to insufficient data. For the phases *resource extraction/energy supply, material refinement*, and *recycling/disposal*, generic data sets from the ecoinvent database [34] were used. For the life cycle phases production and production process, primary (recorded during operation) and secondary data (see FSS, Sect. 3) were available.

The inputs (i) and outputs (o) are classified in the categories auxiliaries, utilities, electrical energy, equipment and residuals in accordance to the classification presented by Wesche et al. [32] (Fig. 3). Auxiliaries include materials,

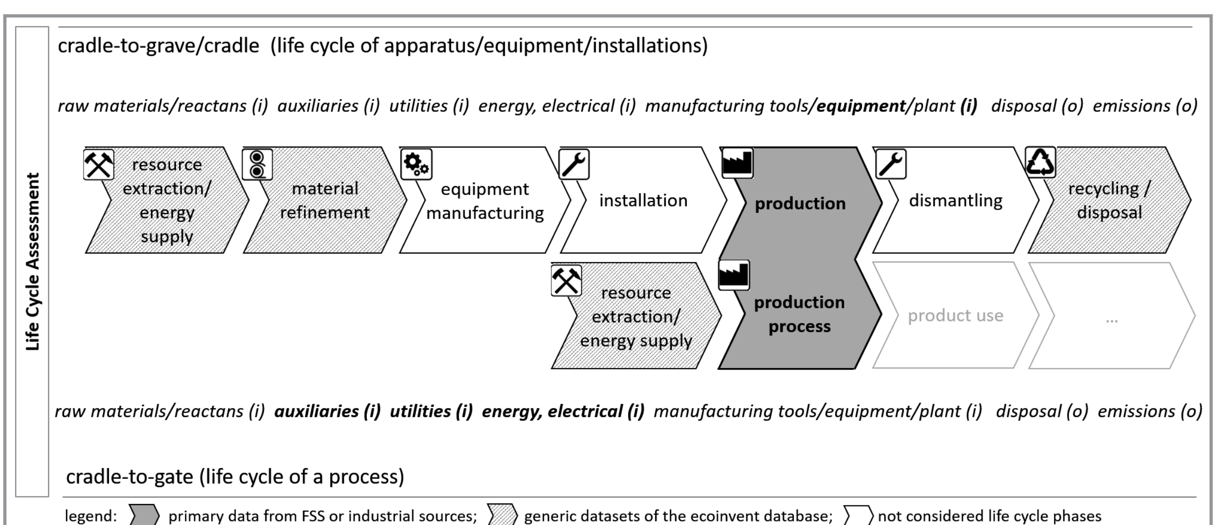

Figure 3. Combination of considered life cycle phases of apparatus and production process for the ecological assessment (shown in grey) as well as considered inputs (i) and outputs (o) in bold black.

which are part of a process recipe and necessary for the realization of a unit operation without being part of the product, e.g., solvents for the extraction of value components in a material converting process. The category utilities covers, e.g., heating media, inert gases, lubricants – materials which are necessary to operate a manufacturing process. Electrical energy represents the electricity which is consumed by, e.g., pumps or compressors. The equipment includes the mass and type of the used material for construction of the apparatus or internals (e.g., droplet separator) as well as their maintenance, as proposed in the ILCD-Handbook [20]. The output residues records amongst others waste, wastewater, by-products or chemical residues in plant equipment components.

The inputs in Fig. 4 highlighted in bold show significant numerical differences in the direct case comparison. These flows are closely related to the influence of entrainment or expenditures due to its prevention. Primary data from flowsheet simulation or industrial sources are supplemented by generic datasets of the ecoinvent database. Since the focus of this study lies on apparatus expenditures associated with its life cycle for a predefined process task, not all inputs/outputs of the phase *production/production process* are considered. This comprises the reactants, process-induced emissions and the product itself, since the synthesis is unaffected by the purification steps for the synthesis gas.

For the ecological assessment, the functional unit is defined as 8000 operational hours, equaling a continuous production period of one year. The assessment is conducted by characterization models of ReCiPe2008 (H) [35], based on datasets from ecoinvent v3.6.

For the assessment the following assumptions were made: The column K1 with and without droplet separator as well as the additional purification step required in the current state are recorded according to the ILCD-Handbook [20]. This includes both the type and quantity of the equipment material. In order to determine the annual ecological expenditures under consideration of the equipment life cycle, the annual plant-related expenditures are determined according to the approach of Wesche et al. [30]. For this purpose, the procurement as well as maintenance over the useful life and disposal or recycling are recorded. The result is an annual ecological expenditure of 15 % of the total expenditures allocated to the production process. This takes on one hand into account higher maintenance requirements due to prevailing operating and process conditions as well as faster wear and tear and the associated early procurement of spare parts on the other hand.

Not considered in the assessment is the insufficient product flow specification of the current state which even after the recovery of the washing agent still contains 3.6 $t\,h^{-1}$ of methanol, as well as approx. 3.5 $t\,h^{-1}$ of CO_2. In this case, an additional downstream processing would have to be designed. However, this was not part of this study.

4.2.2 Economic Assessment

For the assessment of the economic expenditures the costs over the life cycle of the plant are considered. In Fig. 4 the phases *development, equipment manufacturing, procurement, production*, and *recycling/disposal* [36] are shown. From an operatoŕs point of view the last three phases are relevant and thus are accounted for the life cycle assessment of the case study. This includes the investment, installation costs, maintenance costs, and operational costs as well as separate environmental costs and sales revenues. For this study, a use phase of 30 years is considered.

Investment The investment for the absorber column K1 is calculated based on the short cut design, see Chapter 3. Here, the absorbers in the investigated cases differ mainly due to the inclusion of the additional droplet separator in the column head. This is taken into account by an invest of approximately 13 900 € per droplet separator. Since the life time of the droplet separator is estimated to be 10 years, a total of three eliminators are calculated for the investigations. For the absorber (K1) with packing internals and trays an investment of approx. 1 million € is estimated. The additional purification stage is calculated with an invest of approx. 2 843 000 € for the three HEXs, the flash and the expander. The HEXs are estimated with costs of approx. 400 € m^{-2} heat transfer surface – without installation costs or ancillary equipment, such as instrumentation or piping, etc. For the additional expander and for the flash an investment of respectively 40 000 and 25 000 € are calculated.

Installation In order to estimate the costs for the installation of the apparatuses as well as the necessary ancillary equipment, the approach of cost estimation by Guthrie for the module "Apparatuses and Equipment", as shown in [38], is used. Based on this module, the direct assembly and direct ancillary equipment are determined.

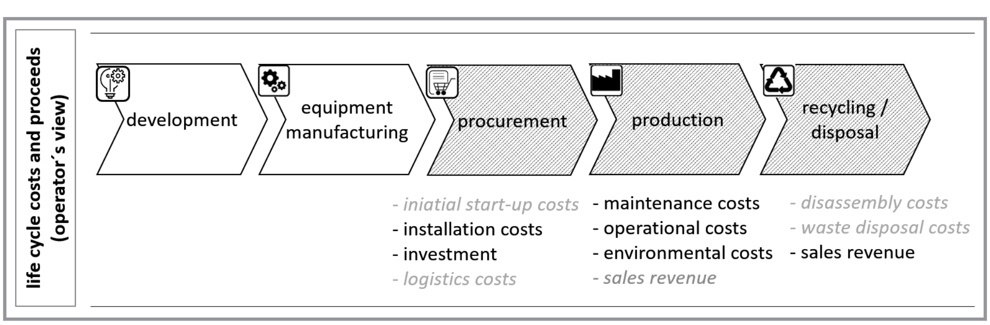

Figure 4. Life cycle phases from the operator's point of view (grey) with different costs types for each phase [39]; black: considered costs, light grey: not considered costs.

Maintenance The maintenance costs are estimated using the maintenance cost rate [39]. For the chemical industry the range is typically between of 1.5 ... 10 % [40–43]. The maintenance cost rate refers to the replacement value on the effective date and takes direct maintenance costs into account. In order to depict the costs for a scheduled production shutdown (petrochemicals every 2 ... 5 years) the expenses for dismantling and cleaning of the equipment are recorded over the estimated number of working hours. To determine the higher degree of apparatus contamination due to entrainment, 32 working hours are assumed for the cleaning of the absorber in the current state as well as further 40 h for the additional purification stage. For the case with droplet separator however, 16 h are estimated. Unscheduled production downtime resulting, among other things, due to the heavy contamination of individual apparatus by droplet entrainment is not considered, although an unplanned production downtime in the petrochemical industry means losses up to millions per day. Among others, this fact will be part of further investigations.

Operation During operation the costs caused by the consumption of utilities as well as the electrical energy demand are taken into account. For the electricity a market price of 0.08 € kWh^{-1} is set. The price for steam at 6 bar(a) is estimated to be 12 € per ton. The expenditures for cooling water and ammonia is calculated on the basis of the electricity demand within the utility cycles. In order to record the expenditures regarding process water for the additional purification stage, a heat integration with an internal process flow originally heated by steam is assumed. Of the associated costs for steam, 40 % are allocated to the process water used here.

Environmental The environmental costs include the expenditures for CO_2-certificates, which were calculated based on the electrical energy demand and steam consumption multiplicated with the characterization factors of the ReCiPe2008 method (electricity: 0.57781 CO_2-Eq./kWh, steam: 0.10252 CO_2-Eq./MJ) [36]. For the certificates the average price of 25.03 € t^{-1} for the time period 04/2019 ... 02/2020 is taken into account [44]. Possibly existing emission certificates were not considered since a comparative assessment has been performed.

Revenues In addition, the revenue from the material sale in the course of dismantling the plant are also included in the analysis. The scrap price is assumed to be 1190 € t^{-1} V4A steel (status: July 14, 2020).

5 Results

Tab. 2 showcases the masses and energy demand of the Recisol process related to 8000 h operation time. The annual quantities of the auxiliary methanol are reduced by 98 % compared to the current state with an entrainment of 1.5 %. The data given here already take into account the additional purification step which separates and recycles approx. 68 % of the entrained detergent quantity.

While a slightly reduced quantity is listed for cooling water, the requirements for thermal energy provided by steam and thermal oil are increased in the case with droplet separator (steam: +1.5 %, ammonium: +0.1 %). This results from the lower mass flow rates in the process for the current state, since in column K1 approx. 11.5 t h^{-1} methanol are entrained. The same applies to the increased demand (+1.4 %) for electrical energy resulting from the operation of the pumps in the process. The heat quantity of process water results from the additional purification step downstream of column K1, which serves to separate the entrained methanol. The indicated equipment masses of the plant include the amount of material used in column K1 and in the current state the additional purification step as described above.

The data show an overall reduction of the utility demand for the simulated Rectisol process of 4 % by using a droplet separator in column K1. Based on these data the life cycle inventory (LCI) is established.

Table 2. Materials and energy taken into account for the case study.

Operation time 8000 h		Unit	Values		
			Current state	With droplet separator	Deviation with drop. separator/ current state [%]
Auxiliaries	Methanol	[$t\,a^{-1}$]	29 096	477	−98.4
Utilities	Cooling water (18 °C)	[$GJ\,a^{-1}$]	282 318	281 802	−0.2
	Ammonium (−36 °C)	[$GJ\,a^{-1}$]	339 416	339 776	+0.1
	Process water (60 °C)	[$GJ\,a^{-1}$]	468 450	0	−100.0
	Steam (6 bar(a))	[$GJ\,a^{-1}$]	8 178 400	8 302 400	+1.5
Energy, electrical		[$kWh\,a^{-1}$]	8 496 724	8 727 523	+1.4
Equipment		[t]	319	100	−68.6

5.1 Life Cycle Assessment

For the ecological assessment life cycle inventory datasets from the ecoinvent database v3.6 [34] are used. The auxiliary "methanol" is represented by "market for methanol". For the utility "steam" the dataset "market for heat, from steam, in chemical industry" is chosen. The expenditures for the supply of cooling water and thermal oil are recorded through the consumption of electrical energy (dataset "market for electricity, medium voltage") of pumps and compressors for the reprocessing in a cooling tower or ammonium evaporator, representing a typical production site of the chemical industry. To assess the ecological impact caused by the considered equipment, the datasets "market for steel, chromium steel 18/8" is chosen.

In Fig. 5 an excerpt of the LCA results for the impact categories *climate change* (CC), *fossil depletion* (FD), *marine ecotoxicity* (MET), and *human toxicity* (HT) are shown. In all four impact categories, the case with droplet separator demonstrates a better ecological performance then the current state. The highest reduction of the potential ecological impact is shown in the impact category FD with –9 %, the lowest one in HT with approx. –3 %. The results also indicate that the decrease is primarily influenced by the reduction of methanol.

In the current state as well as in the case with droplet separator more than 90 % of the ecological expenditures are caused by the provision of the utilities. The reduced amount of utilities, see Tab. 2, additionally decreases the ecological expenditure by up to approx. 3 %.

The heatmap in Fig. 6 represents the results of a focus analysis related to the auxiliaries, utilities, electrical energy and plant expenditures and shows partially high deviations. On the one hand, the differences result from the different material and energy requirements of the current state and the case with droplet separator (Fig. 6). On the other hand, this is due to the different ecological weighting of the individual substances depending on the impact category under consideration. Especially the steam consumption causes between 83 and 92 % of the ecological expenditures in the impact categories CC and FD. The influence in the other two categories is more evenly distributed between steam, ammonium and cooling water consumption – here the share vary between 23 and 45 %. The latter two of the utilities cause only approx. 3 to 7 % in the impact categories CC and FD.

Obviously, the consideration of only a single environmental problem area, as the often in public discussions used impact category climate change, does not do justice to the multi-dimensional problem of environmental assessment since it implies the risk of improving production processes in a single impact category at the expense of other impact categories. The four here presented impact categories are an expert of the assessment and consider typical environmental impacts of the chemical industry due to the use of a variety of solvents and a high consumption of fossil resources for the solvents as well as heating and cooling operations.

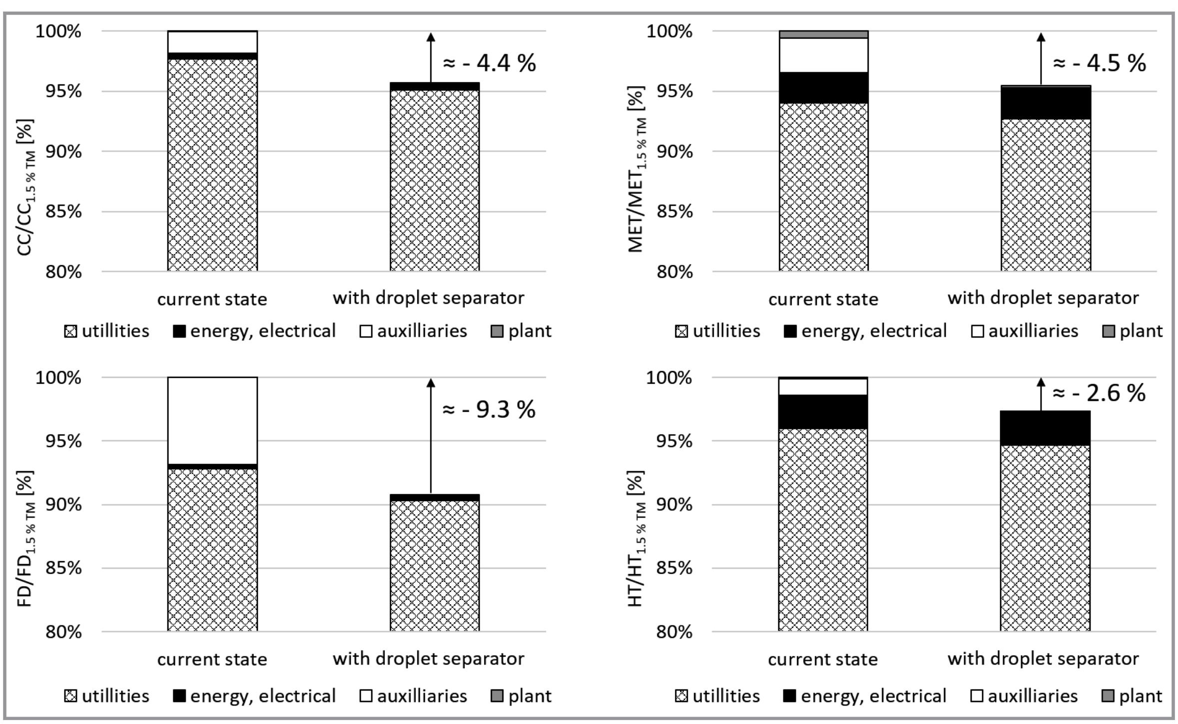

Figure 5. Ecological impact of the Rectisol process for the current state (entrainment 1.5 %) as well as the case with droplet separator (entrainment 0 %) – results of the impact categories *climate change* (CC), *marine ecotoxicity* (MET), *fossil depletion* (FD), and *human toxicity* (HT) calculated by using the characterization models of the ReCiPe2008 method [35].

LCA fE= 8,000 h		CC [t CO2-Eq.] current state	CC [t CO2-Eq.] with drop. separator	MET [t 1,4-DCB-Eq.] current state	MET [t 1,4-DCB-Eq.] with drop. separator	FD [t oil-Eq.] current state	FD [t oil-Eq.] with drop. separator	HT [t 1,4-DCB-Eq.] current state	HT [t 1,4-DCB-Eq.] with drop. separator
auxilliaries	methanol	1.9%	0.03%	2.9%	0.1%	6.9%	0.1%	1.3%	0.02%
utillities	cooling water	4.6%	4.7%	22.9%	23.8%	3.0%	3.2%	23.6%	24.0%
	ammonium	5.5%	5.7%	27.5%	28.7%	3.6%	3.9%	28.3%	28.9%
	process water	2.4%	0.0%	1.2%	0.0%	2.4%	0.0%	1.2%	0.0%
	steam (6 bara)	85.0%	89.0%	42.3%	44.7%	83.8%	92.4%	42.9%	44.4%
energy, electrical		0.5%	0.5%	2.5%	2.7%	0.3%	0.4%	2.6%	2.7%
plant		0.035%	0.011%	0.577%	0.189%	0.023%	0.008%	0.114%	0.037%
ecological expenditures [t x-Eq.]		*985,857*	*956,378*	*6,270*	*6,030*	*416,059*	*382,983*	*174,059*	*170,679*

quantity share [%]
0-5
6-10
11-25
26-40
41-50
51-60
61-75
75-100

Figure 6. Results of the focus analysis in the impact categories *climate change* (CC), *marine ecotoxicity* (MET), *fossil depletion* (FD) and *human toxicity* (HT) using the characterization models of the ReCiPe2008 method [35].

For the current state, the potential ecological impacts of the auxiliaries represent less than 5 % of the overall expenditures in the impact categories *climate change* (CC), *marine ecotoxicity* (MET), and *human toxicity* (HT). In the remaining category *fossil depletion* (FD) a share of approx. 7 % is calculated. The utilities represent the highest influence factor. As already mentioned, in all categories the expenditures caused by the steam consumption account for the biggest share. In the categories HT and MET, the utilities cooling water and ammonium show a similarly high percentage of the ecological expenditures. These vary between approx. 23 and 29 %. The electricity accounts for less than 3 % of the overall expenditures in both current state and the case with droplet separator. The influence of the added apparatuses for the additional purification amounts to max. 0.5 % of the ecological expenditures (impact category MET, current state). The here considered phases of the apparatus life cycle (see Fig. 3) do not show a significant influence on the overall result. This is due to the fact that for the comparison of current state and the case with droplet separator the utilities and auxiliaries are taken into account regarding the complete Rectisol process. However, for the equipment only the deviation in the column K1 and the subsequent purification stage are included. Both are affected by the changes caused by the added droplet separator. Aspects such as a possible upgrade of the downstream equipment resulting in higher separation efficiency or an earlier wear and tear of the equipment due to corrosive effects by entrained droplets are not part of this study and will investigated in future work.

The assumed additional purification step enables the recovery of 2/3 of the entrained methanol. Typical in retrospect installed industrial solutions such as external droplet separators or other disposable "safety apparatus" usually do not enable any form of recovery of the washing agent. For the Rectisol process investigated in this case study, further sensitivity studies show that a total loss of the entrained detergent would significantly affect the results. In such a scenario without any form of methanol recycle in the respective "current case" (1.5 % entrainment) the inclusion of a droplet separator leads to a higher decrease of the ecological expenditures, respectively of –8 % in CC, of –10 % in MET, of –21 % in FD as well as –5 % in HT.

Due to the high share of the utilities in regards to the overall expenditures, sensitivity studies regarding the utility infrastructure from different production sites/locations, a change to other media or electrical heating and cooling are conceivable. The latter option could have far reaching influence on the LCA results in regards to the efforts of government and industry to reduce the greenhouse gas emissions through the use of an electricity mix based on renewable energy. However, for such consideration a reliable data basis is necessary. The implementation of infrastructure data for different operating sites is scheduled for future works.

5.2 Life Cycle Costing

The costs of the considered life cycle phases are calculated based on the assumption mentioned in Sect. 4.2 (economic assessment). The operation of column K1 with a droplet separator results in overall reduced costs of approx. 363 million € over the whole life cycle with a use time of 30 years (Tab. 3). This corresponds to approx. 12 million € per year.

Due to the reduction of the purification step, the costs in the procurement phase for the case with droplet separator are 66 % lower than for the current state. Although the cost reduction in the production phase is much smaller – in percentage terms hovering around 13 % – it nonetheless amounts to a saving of more than 362 million € over the use phase of the production plant. Due to supplementary equipment resulting from the additional purification step, the current state achieves 68 % higher proceeds in the life cycle phase *recycling/disposal*.

The main costs result from the LC phase *production*. In that phase, the operational, maintenance and environmen-

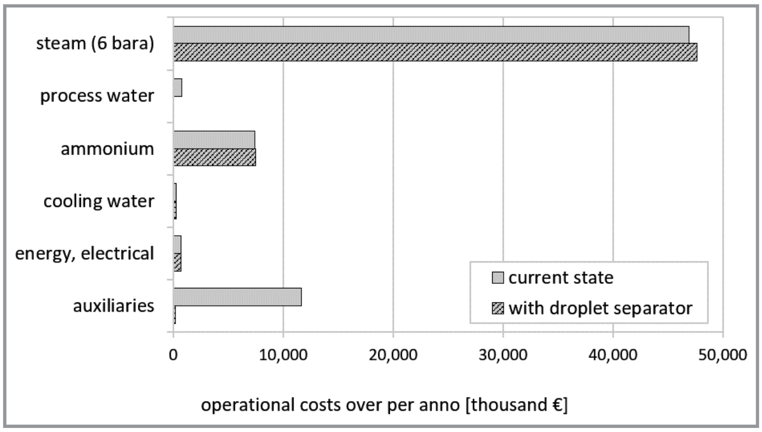

Figure 7. Focus analysis of the operational costs in the life cycle phase *production* for the current state and the case with droplet separator.

tal costs are considered. Out of those three the operational costs account for the biggest share (Tab. 3). Comparing the operational costs between the cases with droplet separator and the current state, a difference of approx. 17 % can be observed, resulting in reduced costs of 347 million € in 30 years.

For the operational costs, the biggest difference results from the cost position of the auxiliaries, respectively the washing agent methanol. The losses caused from the entrainment lead to additional costs of 344 million € over 30 years or 11.4 million € per year (Fig. 7). As in the ecological assessment, the reduction of methanol showcases the highest influence. For this case study, it has to be emphasized that 68 % of the methanol is recovered by the assumed additional purification stage and only about 1/3 of the entrained detergent has to be replaced in the process. Without the additional purification, the share of operational costs would be significantly higher since the costs incurred in this recovery are much lower in comparison, see process water in Fig. 7 as well as the share of investment in Tab. 3.

The additional steam demand of the case with droplet separator (124 000 GJ a^{-1}, see Tab. 2) results in additional costs of 0.7 million € per year. In contrast to that, the costs saved from the operation of the additional purification stage amounts to approx. 0.8 million € per year for the current state.

The environmental costs differ by 1 %, which the case with droplet separator causes less than the current state. This results over in an overall difference of approx. 4.8 million € over 30 years. The difference between the maintenance costs amounts to overall 5.7 million €.

In the production phase the highest costs are recorded but so are the strongest potential from the use of the droplet separator. The downstream purification in the current case is included in the procurement phase (investments and equipment installations) at additional costs of 4.7 million €. This compares to 0.42 million € for the installation of three droplet separators in the head of the column over the expected 30 years. In case of investment decisions, a decision for the droplet separator technology would therefore already have been made in this life cycle phase.

The additional downstream purification considered here for the recovery of the washing agent does not necessarily correspond to the standard solution in industrial applications. Commonly, a moderate overdesign of the column tries to prevent additional external, downstream droplet separators in later operation. Conversely, this leads to higher energy consumption during operation and additional costs that are not directly included in the capex at the time of the decision. Therefore, new technologies are usually not considered due to higher investments. In the case of entrainment as described here, this can have a significant influence on costs over the operation time since in addition to losses of detergent, downtimes due to the occurrence of entrainment are also possible. In the petrochemical industry the latter can entail costs up to several 100 000 to 1 million € per day. With restart times of one till two weeks, the costs quickly add up to tens of million Euros.

For this reason, a holistic view of the life cycle is absolutely necessary for the economic assessment, because

Table 3. Overview of the life cycle costs of the current state and with droplet separator.

Life cycle phase	Cost typ	Current state [mio €]	With droplet separator [mio €]
Procurement	Invest	4.21	1.49
	Installation costs	5.07	1.67
Production	Maintancene costs	8.53	2.87
	Operational costs	2035.76	1689.32
	Environmental costs	722.79	717.94
Disposal	Proceeds	–0.37	–0.12
	Overall costs	2775.99	2413.17

otherwise the potentials offered by a new technology cannot be recognized.

6 Conclusion

The present case study uses the effects of entrainment to address a typical challenge of vapor/liquid separation operations in the process industry. In order to quantify the effects of this phenomenon on the energy efficiency of an apparatus, a 3-stage column for the purification of a C_nC_m-mixture was modelled in a flow sheet simulation, which depicts the entrainment in the feed stream as well as over the individual stages in detail. Based on the variation of the reflux ratio for a fixed product stream composition the additional energy consumption due to entrainment was determined. The difference between no and the highest investigated rate of entrainment amounts up to 37 GJ annually. This results in a saving potential of up to 21 t CO_2-Eq. per year from an ecological point of view in the impact category climate change (ReCiPe2008) for both the condenser (cooling water) and the evaporator (steam, 6 bar).

To quantify the effects of a droplet separation technology in an entrainment-sensitive production process, the Rectisol process was modeled. The results show potential savings of 48 823 t CO_2-Eq. per year in the impact category climate change. This corresponds to savings of approx. 4 % in relation to the total process expenditures. Similar saving potential are also visible in two of the other investigated impact categories - MET and FD. The deviations in the impact category FD are with 9 % twice as high. If only the reportable emissions of the process operators' point of view are taken into account (here utilities and electricity), the saving potential in the impact category climate change amounts up to 25 600 t CO_2-Eq. per year.

In general, the case study shows that for the assessment of new technologies, not only the apparatus or the unit operation alone need to be considered, but also their integration into and resulting effects onto the production process. The economic assessment proves the necessity to consider the entire life cycle. Here, a holistic approach in the preparation of a decision basis not only considers the investment volume but also includes the life cycle phase of production, which is usually associated with significant costs. In order to make a reliable statement on the effects of the entire life cycle of an apparatus, it must be fully recorded and balanced. Further sensitivity studies will address among others the influence of the infrastructure and production downtimes. This was not possible within the context of this study but will be part of future research activities.

The joint project "Drop formation and reduction in mass transfer devices – TERESA" is funded by the Federal Ministry of Economics and Energy (BMWi) as part of the 6th Energy Research Program. The authors thank Linde AG-Linde Engineering devision for the provision of information for the case study as well as Envimac Engineering GmbH for the exemplary process. Open access funding enabled and organized by Projekt DEAL.

Abbreviations

CC	climate change
C_nH_m	carbon hydrogens
Eq.	equivalents
FD	fossil depletion
FSS	flow sheet simulation
HEX	heat exchanger
HT	human toxicity
LCA	life cycle assessment
LCC	life cycle costing
MET	marine ecotoxicity

References

[1] Gesetz zur Einführung eines Bundes-Klimaschutzgesetzes und zur Änderung weiterer Vorschriften in *Bundesgesetzblatt Jahrgang 2019 Teil I Nr. 48*, Bundesanzeiger, Bonn **2019**.

[2] *SPIRE 2050 Vision: Towards the Next Generation of European Process Industries*, A.SPIRE, Brussels **2018**. www.spire2030.eu

[3] P. Tello, R. Weerdmeester, *SPIRE ROADMAP*, A.SPIRE, Brussels **2013**. www.spire2030.eu

[4] R. Geres, A. Kohn, S. Lenz, F. Ausfelder, A. M. Bazzanella, A. Möller, *Roadmap Chemie 2050: Auf dem Weg zu einer treibhausgasneutralen chemischen Industrie in Deutschland*, FutureCamp Climate GmbH, DECHEMA Gesellschaft für Chemische Technik und Biotechnologie e. V, **2019**.

[5] M. Wesche, A. Paschetag, K. Jasch, M. Häberl, S. Scholl, *ChemBioEng Rev.* **2018**, *5 (3)*, 180–191. DOI: https://doi.org/10.1002/cben.201700015

[6] Y. Yao, D. J. Graziano, M. Riddle, J. Cresko, E. Masanet, *Environ. Sci. Technol.* **2015**, *49*, 14704–14716. DOI: https://doi.org/10.1021/acs.est.5b03851

[7] A. Mendoza Beltran, B. Cox, C. Mutel, D. P. van Vuuren, D. Font Vivanco, S. Deetman, O. Y. Edelenbosch, J. Guinée, A. Tukker, *J. Ind. Ecol.* **2018**, *24 (1)*, 64–79. DOI: https://doi.org/10.1111/jiec.12825

[8] C. Liptow, A.-M. Tillman, M. Janssen, *Int. J. Life Cycle Assess.* **2015**, *20*, 632–644. DOI: https://doi.org/10.1007/s11367-015-0855-1

[9] S. Gavankar, S. Suh, A. A. Keller, *J. Ind. Ecol.* **2014**, *19 (1)*, 51–60. DOI: https://doi.org/10.1111/jiec.12175

[10] A. C. Hetherington, A. L. Borrion, O. G. Griffiths, M. C. McManus, *Int. J. Life Cycle Assess.* **2014**, *19*, 130–143. DOI: https://doi.org/10.1007/s11367-013-0627-8

[11] A. G. Parvatker, M. J. Eckelman, *ACS Sustainable Chem. Eng.* **2019**, *7*, 350–367. DOI: https://doi.org/10.1021/acssuschemeng.8b03656
[12] M. Shibasaki, N. Warburg, P. Eyerer, in *Proc. of the 13th CIRP Int. Conf. on Life Cycle Engineering*, Katholieke Universiteit Leuven, Leuven **2006**, 61–64.
[13] F. Piccinno, R. Hischier, S. Seeger, C. Soma, *J. Cleaner Prod.* **2016**, *135*, 1085–1097. DOI: https://doi.org/10.1016/j.jclepro.2016.06.164
[14] T. Hummen, F. Kästner, in *Proc. from the LCA XIV Int. Conf.*, American Center for Life Cycle Assessment, Vashon, WA **2014**, 19–30.
[15] M. Paschetag, Ökologische Bewertung von Verfahren in Mehrzweckanlagen der Prozessindustrie, *Ph.D. Thesis*, Technische Universität Braunschweig **2020**.
[16] *Commission Recommendation of 9 April 2013 on the use of common methods to measure and communicate the life cycle environmental performance of products and organisations*, 2013/179/EU, European Commission, Brussels **2013**.
[17] M. Z. Hauschild, R. K. Rosenbaum, S. I. Olsen, in *Life Cycle Assessment* (Eds: M. Hauschild, R. Rosenbaum, S. Olsen), Springer, Cham **2018**. DOI: https://doi.org/10.1007/978-3-319-56475-3_1
[18] R. Hischier, S. Hellweg, C. Capello, *Int. J. Life Cycle Assess.* **2005**, *10 (1)*, 59–67. DOI: https://doi.org/10.1065/lca2004.10.181.7
[19] H.-J. Althaus, R. Hischier, M. Osses, A. Primas, S. Hellweg, N. Jungbluth, M. Chudacoff, *Life Cycle Inventories of chemicals: Data v2.0*, ecoinvent Report 8, EMPA, Dübendorf **2007**. www.ecoinvent.org
[20] *International Reference Life Cycle Data System (ILCD) Handbook – General Guide for Life Cycle Assessment – Detailed Guidance*, Publications Office, Luxembourg **2010**.
[21] S. Lim, K. T. Lee, *Biofuels, Bioprod. Biorefin.* **2011**, *5 (2)*, 132–150. DOI: https://doi.org/10.1002/bbb.271
[22] H. K. Jeswani, T. Falano, A. Azapagic, *Biofuels, Bioprod. Biorefin.* **2015**, *11 (2)*, 661–676. DOI: https://doi.org/10.1002/bbb.1558
[23] S. Bello, P. Méndez-Trelles, E. Rodil, G. Feijoo, M. Moreira, *Sep. Purif. Technol.* **2020**, *233*, 116056. DOI: https://doi.org/10.1016/j.seppur.2019.116056
[24] T. Grant, T. Beer, P. K. Campbell, D. Batten, *Life Cycle Assessment of Environmental Outcomes and Greenhouse Gas Emissions from Biofuels Production in Western Australia*, Report KN29A/WA/F2.9, CSIRO, Canberra **2008**.
[25] J. L. Manganaro, A. Lawal, *Energy Fuels* **2016**, *30 (4)*, 3130–3139. DOI: https://doi.org/10.1021/acs.energyfuels.6b00207
[26] Z. Xie, B. Subramaniam, *ACS Sustainable Chem. Eng.* **2014**, *2 (12)*, 2748–2757. DOI: https://doi.org/10.1021/sc500483f
[27] O. G. Griffiths, R. E. Owen, J. P. O'Byrne, D. Mattia, M. D. Jones, M. C. McManus, *RSC Adv.* **2013**, *3 (30)*, 12244. DOI: https://doi.org/10.1039/C3RA41900B
[28] A. Paschetag, M. Wesche, H. Nieder, S. Scholl, *Procedia CIRP* **2016**, *48*, 532–537. DOI: https://doi.org/10.1016/j.procir.2016.03.154
[29] L. Grundemann, Zur Umstellung von chargenweise betriebenen Mehrproduktanlagen auf kontinuierliche Kampagnenfertigung, *Ph.D. Thesis*, Technische Universität Braunschweig, Cuvillier, Göttingen, **2013**.
[30] M. Wesche, M. Häberl, M. Kohnke, S. Scholl, *Chem. Ing. Tech.* **2015**, *87 (3)*, 203–215. DOI: https://doi.org/10.1002/cite.201400086
[31] A. L. Kohl, R. Nielsen, *Gas Purification*, 5th ed., Gulf Professional Publishing, Houston TX **1997**, 1215–1223.
[32] *Syngas Deacification with Rectisol Process*, ProSim, Labège, France, **2015**. www.prosim.net
[33] www.chemstations.com (Accessed on October 24, 2020)
[34] www.ecoinvent.org (Accessed on October 24, 2020)
[35] M. Goedkoop, R. Heijungs, M. Huijbregts, A. De Schryver, J. Struijs, R. van Zelm, *A life cycle impact assessment method which comprises harmonised category indicators at the midpoint and the endpoint level*, Report I: Characterisation, 1st ed., Ministerie van VROM, The Hague **2013**. www.rivm.nl
[36] T. Spengler, C. Herrmann, *Stoffstrombasiertes Supply Chain Management in der Elektro(nik)industrie zur Schließung von Materialkreisläufen*, VDI Reihe 16, Technik und Wirtschaft Nr. 169, VDI, Düsseldorf **2004**.
[37] C. Herrmann, Ganzheitliches Life Cycle Management, *Habilitation*, Technische Universität Braunschweig, Springer, Berlin **2010**.
[38] U. Strauch, Modulare Kostenschätzung in der chemischen Industrie. Konzept eines integrierten Systems zur Abschätzung und Bewertung des Kapitalbedarfs für die Errichtung einer chemischen Anlage, *Ph.D. Thesis*, Technische Universität Berlin **2008**.
[39] *Selection and formation of indicators for maintenance*, VDI guideline 2893, Beuth, Berlin **2006**.
[40] M. März, N. Blechschmidt, L. Weck, *Projektstudie Chemie und Pharmazie: Wertorientiertes Instandhaltungs- und Asset Management*, ConMoto, München **2014**. www.silo.tips/download/projektstudie-chemie-und-pharma
[41] W. Becker, F. Brinkmann, *Kostenrechnung für die Instandhaltung: Ergebnisse einer empirischen Untersuchung*, Otto-Friedrich-Universität Bamberg, Bamberg **2000**.
[42] W. Kern, *Industrielle Produktionswirtschaft*, Schäffer-Poeschel, Stuttgart **1992**.
[43] *Instandhaltungs-Kennzahlen 3*, dankl+partner, Walserberg, Austria **2003**. www.delta-q.de/export/sites/default/de/downloads/ih_kennzahlen_3.pdf
[44] www.finanzen.net/rohstoffe/co2-emissionsrechte/ (Accessed on October 24, 2020)

Chemie Ingenieur Technik

DOI: 10.1002/cite.202000255

Life Cycle Analysis: Assessment of Technologies for Droplet Separation – A Case Study

Mandy Paschetag, André Paschetag, Florian Merkel, Christian Mehringer, Stephan Scholl*

Research Article: A case study is used to investigate the influence of droplet entrainment on energy demand and resource consumption of a single apparatus and on a production process. Based on the mass and energy balances of flow sheet simulation models, the application of a separation technology is assessed from an ecological (LCA) and economic (LCC) perspective.