



Data Article

Life cycle inventory data generation by process simulation for conventional, feedstock recycling and power-to-X technologies for base chemical production



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ABSTRACT

The article presents the methodology and applicable data for the generation of life cycle inventory for conventional and alternative processes for base chemical production by process simulation. Addressed base chemicals include lower olefins, BTX aromatics, methanol, ammonia and hydrogen. Assessed processes include conventional chemical production processes from naphtha, LPG, natural gas and heavy fuel oil; feedstock recycling technologies via gasification and pyrolysis of refuse derived fuel; and power-to-X technologies from hydrogen and CO₂. Further, process variations with additional hydrogen input are covered.

Flowsheet simulation in Aspen Plus is applied to generate datasets with conclusive mass and energy balance under uniform modelling and assessment conditions with available validation data. Process inventory data is generated with no regard to the development stage of the respective technology, but applicable process data with high technology maturity is prioritized for model validation. The generated

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inventory data can be applied for life cycle assessments. Further, the presented modelling and balancing framework can be applied for inventory data generation of similar processes to ensure comparability in life cycle inventory data.

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Specifications Table

Subject	Chemical Engineering: Process Chemistry and Technology
Specific subject area	Chemical technology modelling and balancing for application in life cycle assessment
Type of data	Table
How data were acquired	Process modelling in Aspen Plus V11 Process balancing in MS Excel
Data format	Raw
Description of data collection	Inventory data is generated by generation of validated process models and process chain modelling in Aspen Plus. Process chain modelling and balancing is performed uniformly for conventional, waste-based and CO ₂ -based process pathways.
Data source location	Applied source data is cited in the DiB article.
Data accessibility	With the article
Related research article	F. Keller, R.L. Voss, R.P. Lee, B. Meyer, Life cycle assessment of global warming potential of feedstock recycling technologies: Case study of waste gasification and pyrolysis in an integrated inventory model for waste treatment and chemical production in Germany, Resources, Conservation and Recycling 179 (2022) 106106. https://doi.org/10.1016/j.resconrec.2021.106106

Value of the Data

- Disintegrated LCI data for LCA of chemical processes are sparsely available due to varying degree of process aggregation, allocation to products and balancing boundaries. Inventory data from LCA databases is largely non-transparent about its specific origin and balancing conditions. The provided data give a set of disaggregated process balances generated under uniform and transparent conditions to ensure comparability. The addressed assessment framework provides applicable conditions for process modelling and balancing for generation of process inventories with high comparability.
- The life cycle inventory data can be applied by LCA practitioners.
- The data can be applied by LCA practitioners to generate LCI for base chemical production from conventional and alternative processes under adaptable LCA conditions. Further, provided process modelling assumptions can be applied for process modelling of similar processes to generate comparable LCI.

1. Data Description

The assessed production pathways are illustrated for clarification in Fig. 1. The subsequent section contains an overview of the applied process models, descriptions of the individual processes and the assumptions of process chain balancing. Further data is given in the provided supplementary material. Table S1 gives an overview of the evaluated process pathways and the respective applied process steps. Table S2 to S4 show the generated inventory data for conven-

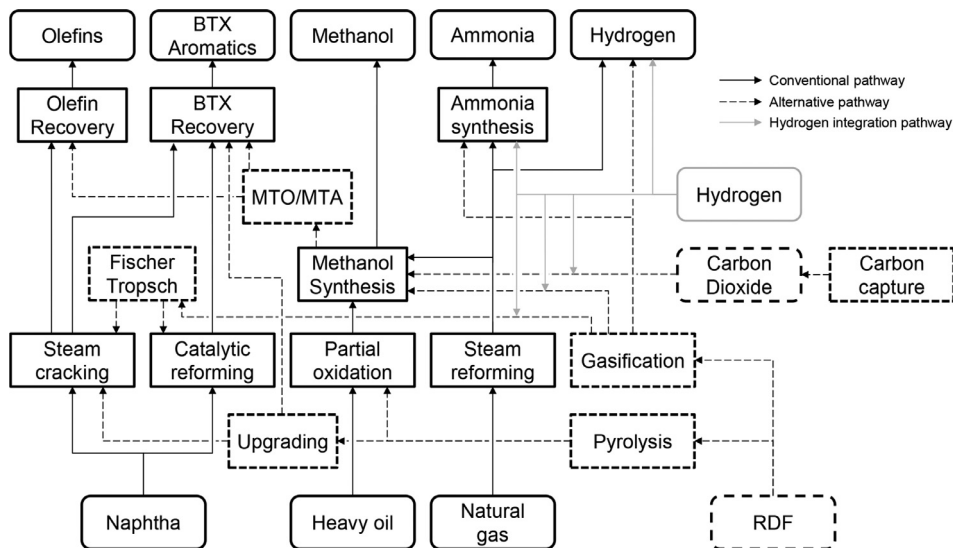


Fig. 1. Illustration of the assessed technologies and base chemical production pathways.

tional, feedstock recycling and PTX production pathways. Further specifics of the applied process models are given in Table S5 to S8, including modelling assumptions, applied performance indicators, applied property methods in Aspen Plus and compositions of solid and liquid materials.

2. Experimental Design, Materials and Methods

Inventory data was generated by process modelling in Aspen Plus V11. Consistent mass, energy and element balances are maintained. Primarily, adaptable individual process models were designed and validated with available experimental and industrial process data. Individual process models were combined and adjusted to design process chain models for the development of complete conversion chains from uniform predefined feedstock to uniform base chemical products.

2.1. Individual process models

An overview of all applied individual process models is given in Table 1. In the following, the processes and modeling approach are introduced individually.

Table 1
Overview of applied individual process models.

Process	Feedstock	Main product	Side product
Steam cracking	Naphtha, LPG	Cracker gas (olefin-rich)	
Olefin recovery	Olefin-rich gas	Ethylene, propylene, C4 olefins	Hydrogen, gasoline (BTX-rich), fuel oil, LPG, naphtha, fuel gas
Aromatic recovery	BTX-rich stream	BTX aromatics	Raffinate (paraffin-rich)
Steam reforming	Natural gas	Raw syngas	
Partial oxidation	Fuel oil, pyrolysis oil	Raw gas	
Quench & scrubber	Raw gas	Raw syngas	
CO shift	Raw syngas	Converted syngas	
Acid gas removal (physical)	Converted syngas	Syngas	Claus gas
Acid gas removal (chemical)	Converted syngas	Syngas	
Carbon capture (chemical)	Flue gas	CO ₂	
Sulphur recovery (Claus)	Claus gas	Sulphur	
Sulphur recovery (liq. ph.)	Off gas (H ₂ S-rich)	Sulphur	
Methanol synthesis	Syngas (CO, CO ₂ , H ₂)	Methanol	
Ammonia synthesis	Syngas (N ₂ , H ₂)	Ammonia	
Catalytic reforming	Naphtha	Reformate (BTX-rich)	Hydrogen, LPG, fuel gas
Methanol-to-Olefins (MTO)	Methanol	Product gas (olefin-rich)	
Methanol-to-Aromatics (MTA)	Methanol	Reformate (BTX-rich)	Hydrogen, fuel gas
Fischer-Tropsch synthesis	Syngas	FT crude	Hydrogen, fuel gas
Gasification	RDF	Raw syngas	
Pyrolysis	RDF	Pyrolysis oil	
Oil upgrading	FT crude, Pyrolysis oil	Naphtha/gasoline (BTX-rich)	LPG, Hydrogen, fuel gas

2.2. Steam cracking

Steam cracking is a pyrolysis process without additional reaction medium, added steam is used for process moderation and reduction of coking. The most relevant feedstock is naphtha, but the range of industrially applied feedstock includes liquefied gases (from ethane), LPG to hydrogenated heavy oils. Depending on the feedstock, the product spectrum also varies (light olefins, hydrogen, aromatics). The steam cracking process is heated by firing of natural gas or fuel gas from subsequent product fractionation.

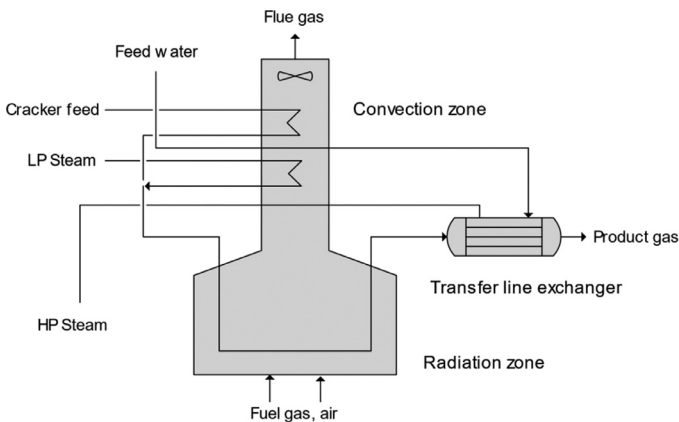


Fig. 2. Visualization of the steam cracking process.

2.3. Olefin product processing

The olefin processing unit consists of a two-stage quenching and liquid separation section, product gas compression, caustic scrubbing for removal of remaining sour gases as CO₂, and multi-stage product gas fractionation section for the supply of high-purity olefin product gases. Depending on production technology and product gas composition, different plant components are required (see Table 2). Process steps for C4 olefin recovery show significant complexity and consequently high modelling demand, despite a limited impact on the overall process balance. Therefore, C4 olefin recovery is considered based on KPIs.

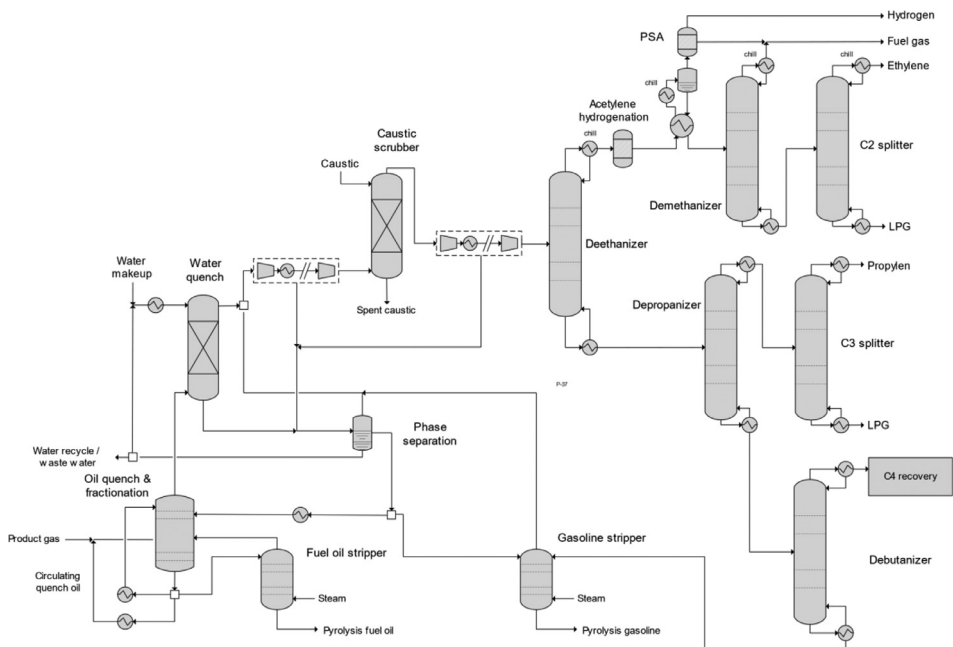


Fig. 3. Visualization of the olefin recovery process.

Table 2
Process element demand by feed for the olefin recovery process.

Primary production technology	Steamcracking		MTO
	Naphtha	LPG	
Oil quench	X		
Water scrubber	X	X	X
Phase separation	X	X	
Aromatic separation	X		
Acid gas removal	X	X	X
Deethanizer, Demethanizer	X	X	X
Hydrogen recovery	X	X	
C2-Splitter, Depropanizer / C3 Splitter, Debutanizer/ C4 Recovery	X	X	X

2.4. Aromatic product processing

The objective of the aromatic processing unit is the separation of non-aromatic compounds, BTX product yield adjustment and BTX purification. An overview of integrated process steps is presented in Table 3. Aromatic extractive distillation and p-xylene adsorption are not modelled due to high modelling demand, but instead considered by KPIs.

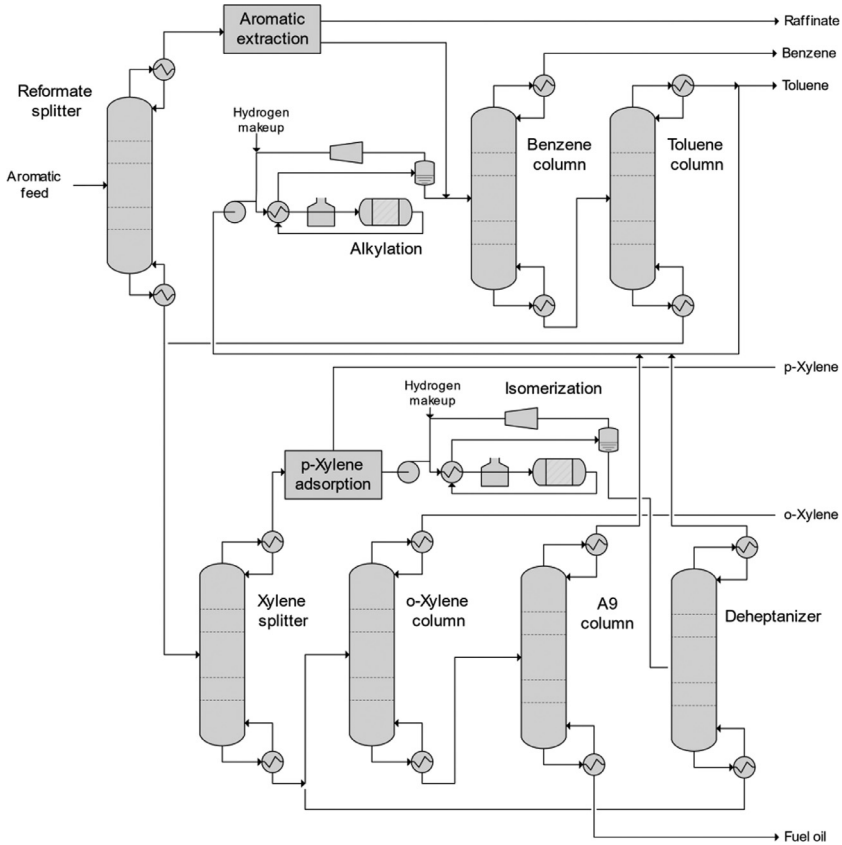


Fig. 4. Visualization of BTX aromatic recovery process.

Table 3 Overview of BTX aromatic recovery process steps.

Process	Extractive distillation	Transalkylation	p-xylene adsorption	Isomerization
Feed	Reformat	Toluene, C10+ aromatics	Xylene mix	m-Xylene, Ethylbenzene
Product	Aromatic mix	Benzene, Xylene	p-Xylene	p-Xylene, o-Xylene
Temperature		430 °C		390 °C
Pressure		35 bar (hydrogen atm.)		17 bar (hydrogen atm.)
Model approach	KPI	Reaction stoichiometry	KPI	Reaction stoichiometry

2.5. Steam reforming

Catalytic steam reforming is the most widespread process worldwide for the production of synthesis gas and is primarily used for the production of hydrogen and ammonia. The process is heated by firing of natural gas or alternative fuel gases. Further the reformer process configuration and reforming conditions depend on the applied feedstock and the target product (see Table 4).

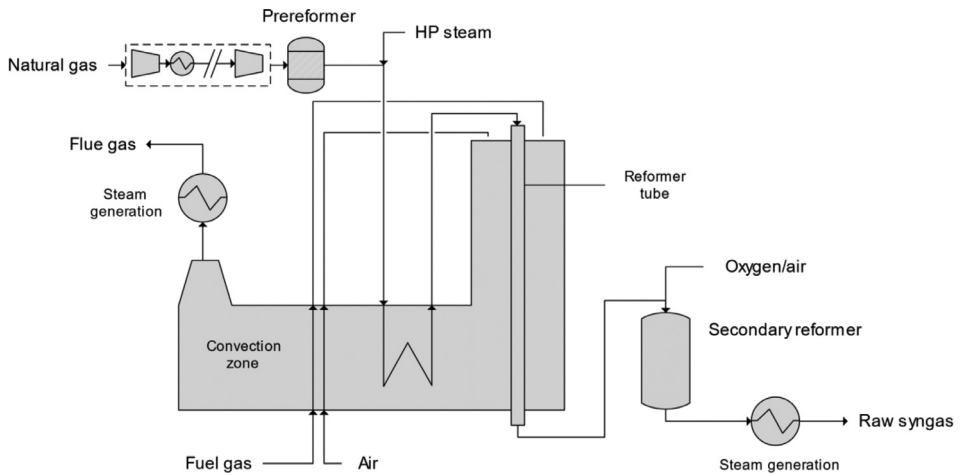


Fig. 5. Visualization of the steam reforming process.

Table 4

Overview of process configuration depending product for steam reforming process.

Product	Hydrogen	Methanol	Ammonia
Reformer pressure	25 bar	25 bar	35 bar
Reformer temperature	850°C	750°C	800°C
Steam/carbon ratio (molar)	3.0	2.5	3.5
Secondary reformer agent	-	Oxygen	Air
Secondary reformer objective	-	$\frac{H_2-CO_2}{CO+CO_2} = 2.05$	$\frac{H_2+CO}{N_2} = 3.0$
Sources		[1,2]	

2.6. Oil partial oxidation

The partial oxidation (POX) of heavy oil and liquid residues is an alternative process of synthesis gas production. In addition to petroleum-based heavy oil, other liquid hydrocarbons such as pyrolysis oil or natural gas can also be used. The produced raw syngas contains soot, which is recovered in the subsequent quenching section and recycled to the POX process.

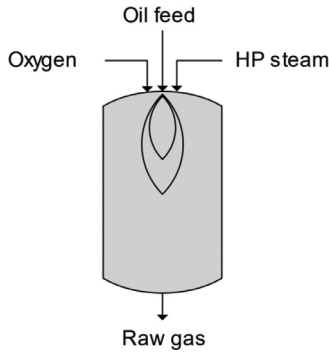


Fig. 6. Visualization of the partial oxidation process.

2.7. Water quench and scrubbing

Gasification and partial oxidation processes require cooling of the raw gas after the primary synthesis gas production as well as the removal of solid particles (in the form of slag or fly ash), tar/oil loads and water-soluble corrosive gas components (especially HCl, NH₃). The used wash water is integrated over both washing steps to limit the fresh water demand and waste water production. Solved gas fractions and tar/oil are recovered by decompression and phase separation. Tar/oil is recycled to the gasification or partial oxidation process. The water recycle pH value is adjusted by caustic addition. Chloride loading is limited by waste water extraction.

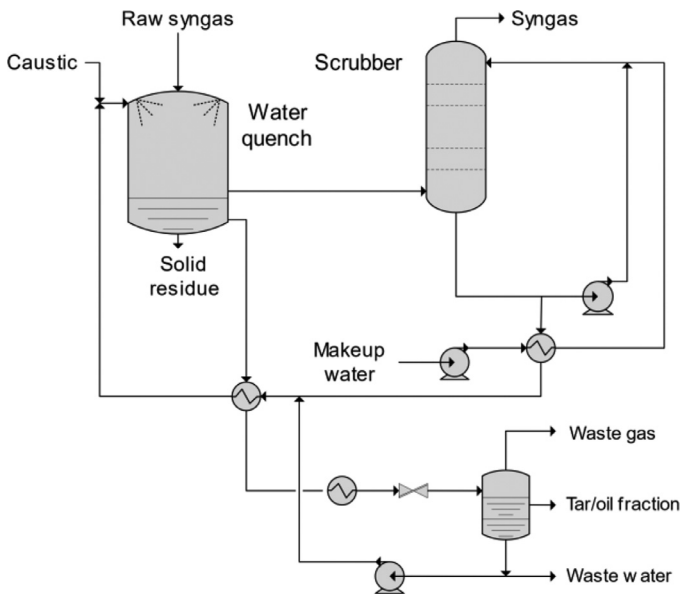


Fig. 7. Visualization of the water quench and scrubber process.

2.8. CO shift

The H₂-CO ratio of the syngas is adjusted by two-stage catalytic conversion in adiabatic fixed bed reactors. CO conversion and bypass depend on the raw gas composition and the type of synthesis gas utilization (maximum conversion for hydrogen and ammonia, partial conversion for methanol, SNG and fuel synthesis). Furthermore, the process is used for the hydrolysis of HCN and COS present in the syngas.

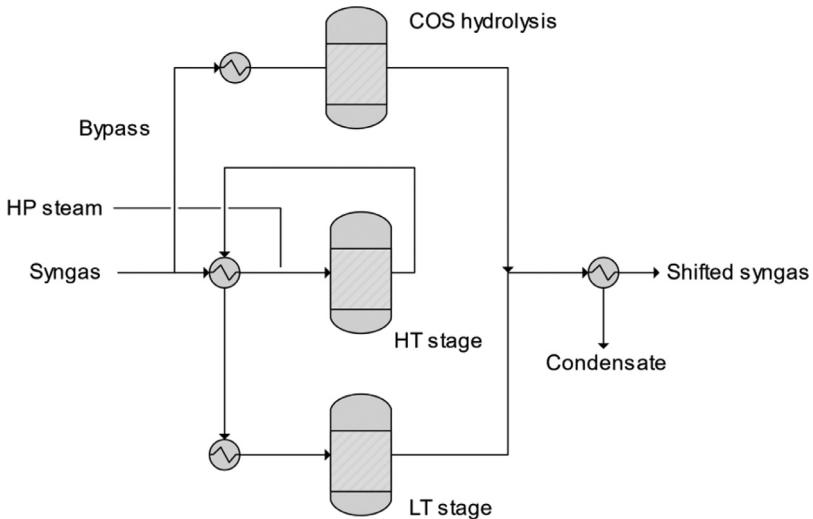


Fig. 8. Visualization of the CO shift process.

2.9. Acid gas removal

Sour gases (especially CO₂ and H₂S) must be removed before syngas utilization. For large-scale industrial applications, a selective physical AGR process with low-temperature methanol is used for this purpose, in which H₂S is recovered separately in high concentration (Claus gas) for subsequent sulfur recovery. CO₂ is recovered in high purity (further referred to as concentrated CO₂) and can be applied as flushing gas or as feedstock in PTX applications. For small-scale applications and low-sulfur feedstocks, but also for CO₂ capture from flue gases, chemical scrubbing agents like amine solutions are applied with downstream residual gas desulfurization (if necessary).

2.10. Sulphur recovery

H₂S separated from syngas is converted to elemental sulfur in a Claus process and can thus be used as a raw material in the chemical and building materials industry. The conversion takes place in a thermal stage for partial oxidation to SO₂ and in three adiabatic catalytic stages for sulfur production with subsequent separation. The third catalytic stage is operated below the sulfur dew point to achieve high sulfur recovery, therefore practical operation requires frequent catalyst regeneration, which is not considered in the simulation. The application of sulfur recovery depends on the H₂S content of the residual gas. If the H₂S content is above 50 vol.-%, the process is carried out as a full-flow process, below 50 vol.-% with a partial bypass flow around the thermal process stage.

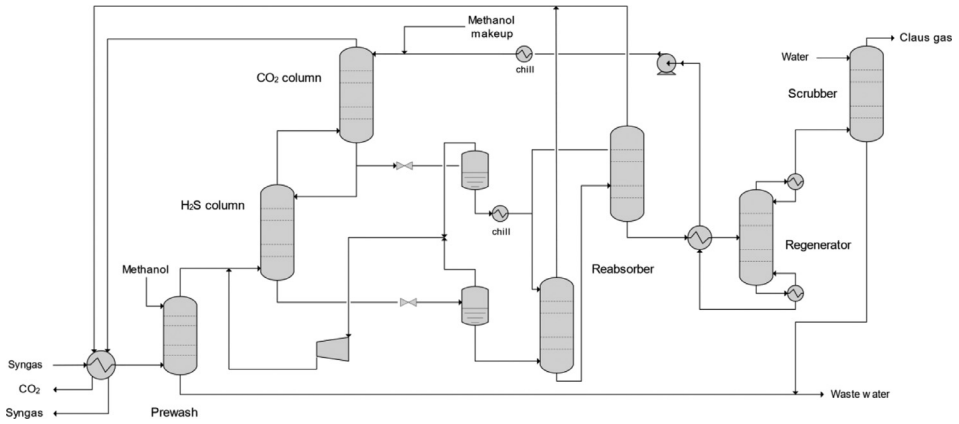


Fig. 9. Visualization of the physical absorption process.

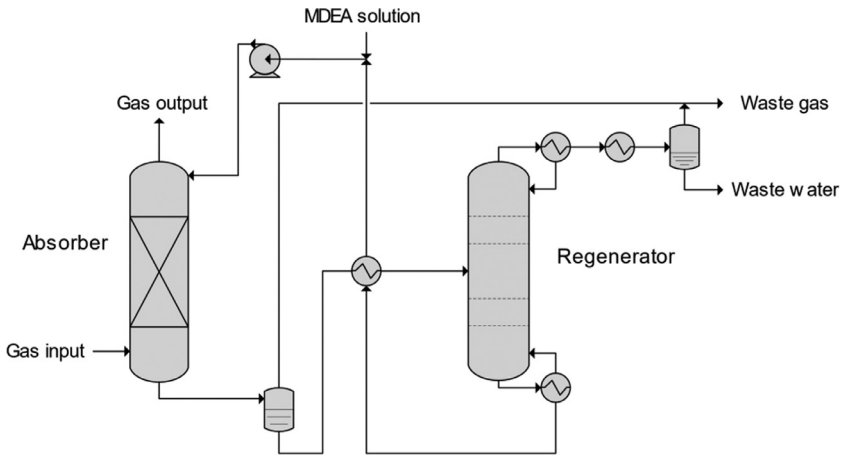


Fig. 10. Visualization of the chemical absorption process.

For low-sulfur streams (below 15 vol.-%) or selective sulfur recovery an iron chelate-based liquid phase oxidation process is assumed. Due to the significant modelling complexity and limited impact on the overall process balance, the process is not modelled in detail but considered by KPIs.

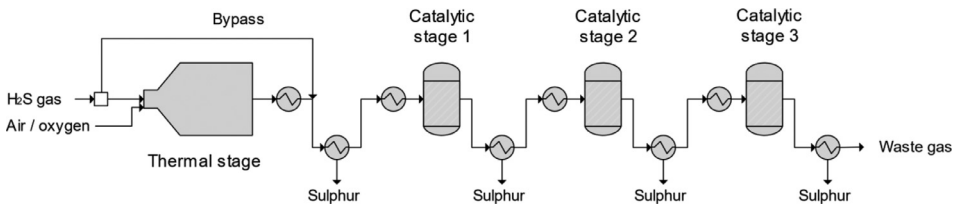


Fig. 11. Visualization of the Claus process.

2.11. Methanol synthesis and purification

Methanol synthesis is an exothermic catalytic reaction, that is realized in an isothermal multi-tubular fixed-bed reactor with boiling water temperature control. Single pass conversion is limited, so the unconverted reactant gas is recycled. The illustrated process design is applicable for syngas as well as for a CO_2/H_2 mixture. Plant-related differences (esp. increased water tolerance of the catalyst) do not influence the process model in the applied modeling depth. The distillative purification of product methanol takes place in two stages.

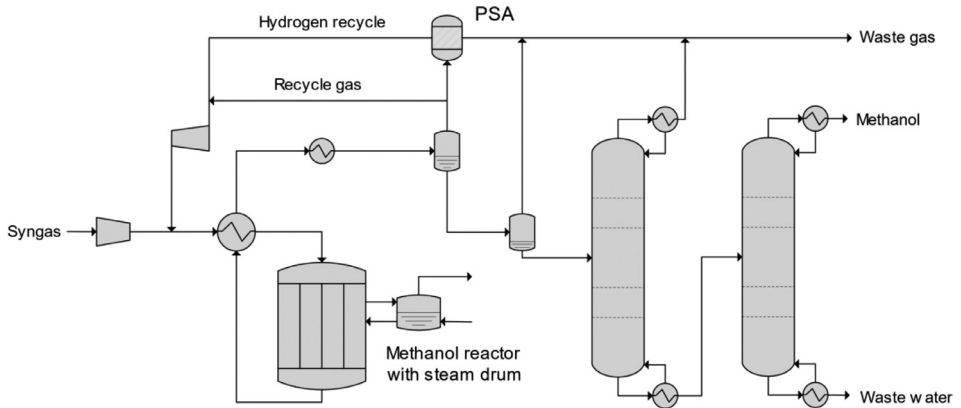


Fig. 12. Visualization of the methanol synthesis process.

2.12. Ammonia synthesis

The Haber-Bosch process for ammonia production is a high-pressure catalytic process, that is realized in an adiabatic fixed-bed reactor with staged reactant feeding. Before compression, any residual traces of CO, CO_2 and oxygen contained in the syngas must be removed by an adiabatic methanation stage. The resulting methane content influences the cycle ratio in the cryogenic cycle and must therefore be individually adjusted depending on the feed gas. Due to high process pressure and cooling requirements, ammonia synthesis is characterized by a significant power demand.

2.13. Catalytic reforming

Catalytic reforming is a standard process in conventional petroleum processing for upgrading of naphtha fractions to gasoline, but is also applied for BTX production. The reforming reaction is an endothermic catalytic reaction, performed in a three-staged moving bed reactor with intermediate gas heating in a fired furnace. Formed coke on the catalyst is continuously burned off. Hydrogen atmosphere is maintained by partial recycling of the formed gas fraction.

2.14. Methanol-to-olefins (MTO)

The oligomerization of methanol to olefins is a catalytic exothermic reaction, that is performed in a fluidized bed reactor with steam atmosphere for moderation. Methanol is converted primarily to dimethyl ether and subsequently to a product gas mixture of mainly olefinic and

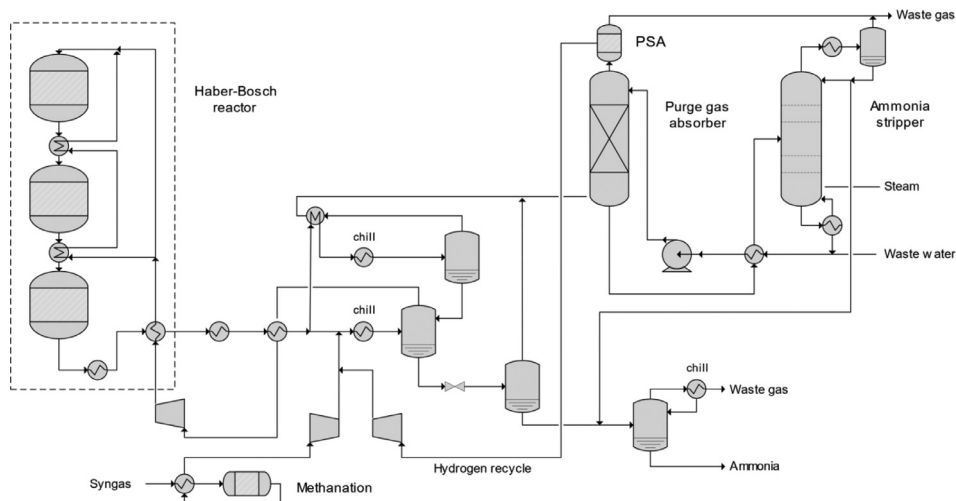


Fig. 13. Visualization of the ammonia synthesis process.

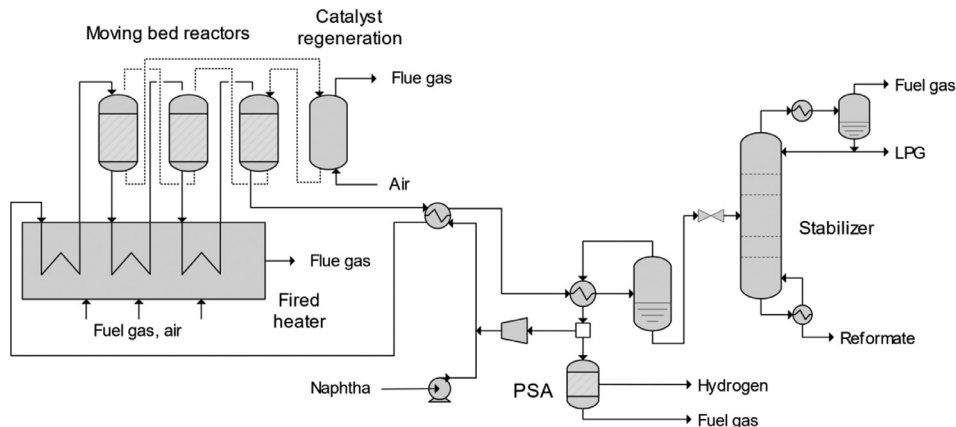


Fig. 14. Visualization of the catalytic reforming process.

paraffinic components up to C5. The reaction temperature is regulated by steam generation. Due to a strong coking tendency on the reactive surface, the catalyst is continuously extracted and regenerated in a regeneration reactor by carbon burn-off with air. The MTO process has a high technology maturity and is applied on large industrial scale in coal-based chemical production facilities in China.

2.15. Methanol-to-aromatics (MTA)

Similar to MTO, the MTA technology was recently primarily developed in China for coal-based chemical production. The process was applied in a demonstration-scale facility, the TRL is about 7. The aromatization process is a catalytic exothermic reaction, realized in a fluidized bed reactor with steam generation for temperature control, similar to the MTO reactor. The product gas is processed similar to a conventional olefin recovery. The C3+ fraction and the non-aromatic fraction from aromatic recovery are recycled to a secondary reactor stage (LHTA). The paraffin

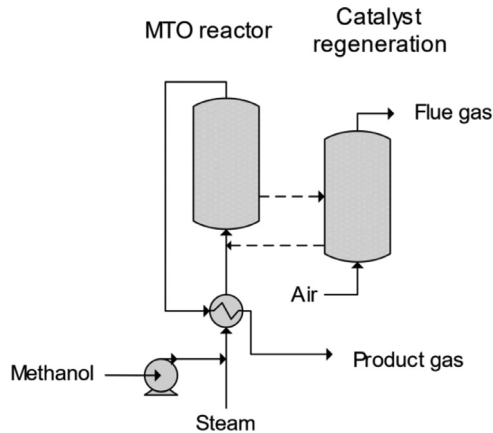


Fig. 15. Visualization of the methanol-to-olefin process.

aromatization process is endothermic and requires preheating. The catalyst is applied in the LHTA stage before the MTA stage due to the higher coking tendency, and subsequently regenerated by carbon burn-off with air.

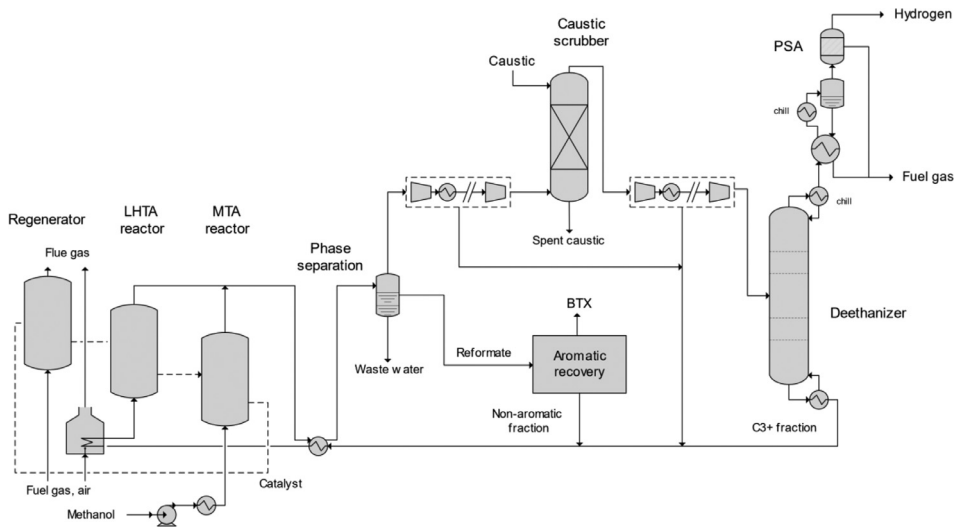


Fig. 16. Visualization of the methanol-to-aromatics process.

2.16. Gasification

For syngas generation from RDF, fixed-bed gasification with liquid slag extraction (BGL type) is modelled. The technology was developed and applied on industrial scale for coal gasification. It was further applied at SVZ Schwarze Pumpe for the production of methanol from a mixture of RDF, plastic waste, wood, tar, sludge and coal [2,3]. The technology was not demonstrated for the processing of unblended RDF until now, but is assumed feasible for this investigation. Gasification feedstock is entered at the reactor top and contacted with the gasification agent counter-

Table 5

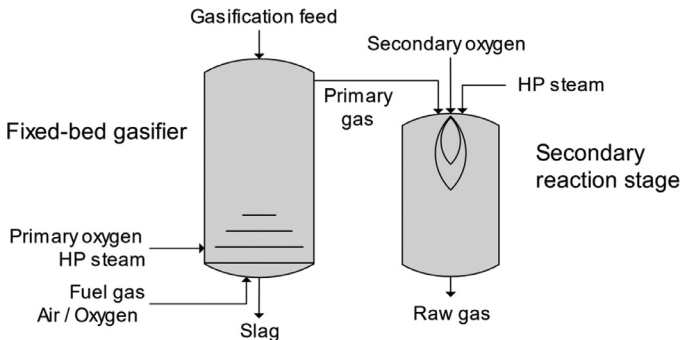
Process characteristics for the fixed-bed slagging gasification process.

		Validation Case [3,6]	Modeling resultswithout post gasification	Modeling results with post gasification
Feedstock				
LHV	MJ/kg (waf)	20.5	23.1	23.1
Volatile Yield	wt.-% (waf)	0.79	0.76	0.76
Ash yield	wt.-% (waf)	0.18	0.10	0.10
Gasification agent				
Oxygen	m3 (STP)/ kg (waf)	0.19	0.22	0.46
Steam	kg / kg (waf)	0.15	0.19	0.41
Results				
Gas exit temperature	°C	757	750	1050
Syngas Yield	m ³ (STP) / kg (waf)	0.77	0.87	1.76
H ₂ -CO ratio (molar)	-	0.54	0.72	1.26
Cold gas efficiency	-	79.2%	82.1%	83.8%
CH ₄ content	vol.-%, wf, N ₂ -free	21.0	24.0	1.2

currently. The gasification reaction is a non-catalytic, autothermal reaction with the reaction heat being generated by partial oxidation of the gasification feedstock. Mineral and metal components exit the reactor vessel at the bottom, completely oxidized and molten by a ring burner and extracted via a slag quencher. Further technology development includes a secondary reaction stage with secondary gasification agent injection and prolonged residence time by means of an extended freeboard zone or an external downdraft reactor, similar to a gas-based POX reactor. By increasing the reaction temperature via partial oxidation, the product gas quality is increased (lower methane content, higher syngas yield and H₂-CO ratio) [4,5].

2.17. Pyrolysis

Predictive modelling of pyrolysis processes of RDF for liquid production is not possible to the knowledge of the author. Waste pyrolysis is experimentally investigated frequently [7–9]. Process characteristics (i.e. energy demand, product yield and composition) vary significantly, especially depending on the applied feedstock, reactor and reaction type (i.e. catalytic/non-catalytic). Applicable simulation investigations in terms of feedstock and product composition are not available.

**Fig. 17.** Visualization of the gasification process.

The pyrolysis process balancing is thus based on the process balance of an existing pyrolysis facility.

The Carbolig technology [10,11] is applied for process balancing. The catalytic liquefaction process applies low pressure and moderate temperature, as process energy is introduced by means of a slurry turbine, generating heat by friction. RDF feedstock is preconditioned and introduced in circulating oil with dispersed catalyst. Product oil fractions are extracted from the circulating oil as vapor, heavy and solid components are extracted by sedimentation.

2.18. Fischer-Tropsch synthesis

Fischer-Tropsch synthesis is applied on industrial scale for the production of hydrocarbons in a broad boiling range, primarily utilized for liquid fuel production from coal (CTL) and natural gas (GTL). For this assessment, a low temperature Fischer-Tropsch process (LTFT) on a cobalt-based catalyst is considered. The oligomerization reaction is exothermic and is realized in an isothermal multi-tubular fixed-bed reactor with boiling water temperature control. The product composition is represented by the Anderson-Schulz-Flory (ASF) distribution with a chain growth probability that is specific to operation conditions, catalyst and reactor type.

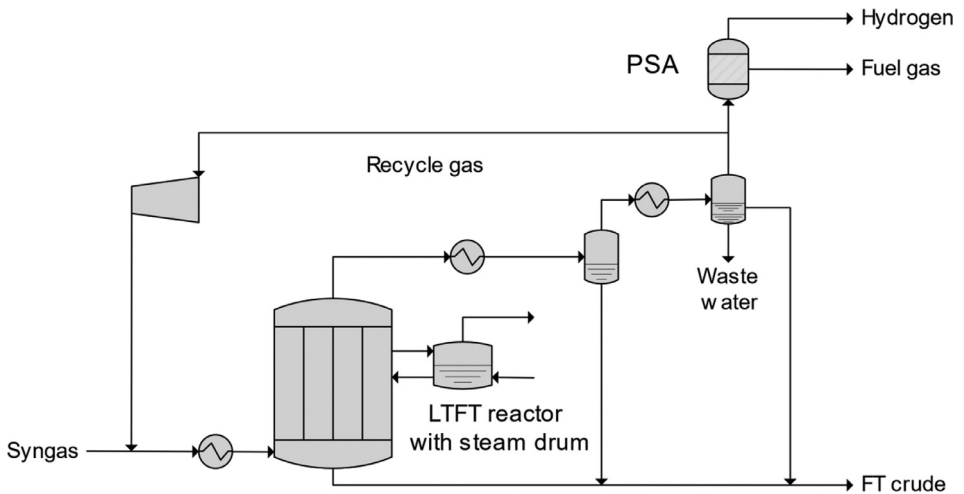


Fig. 18. Visualization of the Fischer-Tropsch process.

2.19. Pyrolysis oil and FT crude upgrading

Product pyrolysis oil contains significant amounts of hetero atoms (esp. oxygen, chlorine, sulfur, nitrogen) and non-paraffinic hydrocarbons, so it needs to be upgraded for application as cracker feedstock. Feed oil is initially catalytically hydrotreated in hydrogen atmosphere for saturation and hydrogenation of hetero atoms. Hydrotreating predominantly results in the hydrogen demand of the upgrading process and is directly associated with the oil composition. Formed waste gas components and CO_2 are removed from the gas fraction by amine scrubbing. Naphtha and LPG are separated in a fractionation step. Heavier oil fractions are recycled to a catalytic hydrocracking step. By kinetic modelling of the hydrocracking reactions the resulting product fraction ratio (Fuel gas, LPG, naphtha) depending on the feed composition and reaction conditions is considered.

Alternatively, upgraded pyrolysis oil is applicable for BTX recovery. Already rich in aromatic compounds, it is possible to selectively convert olefinic and polyaromatic compounds and increase the BTX yield by means of hydrotreating catalyst selection [12,13]. The shown configuration is an adaptation from conventional FT upgrading schemes for liquid fuel production, where a middle distillate fraction is extracted from the fractionation column, isomerized and further fractionated into different fuel types.

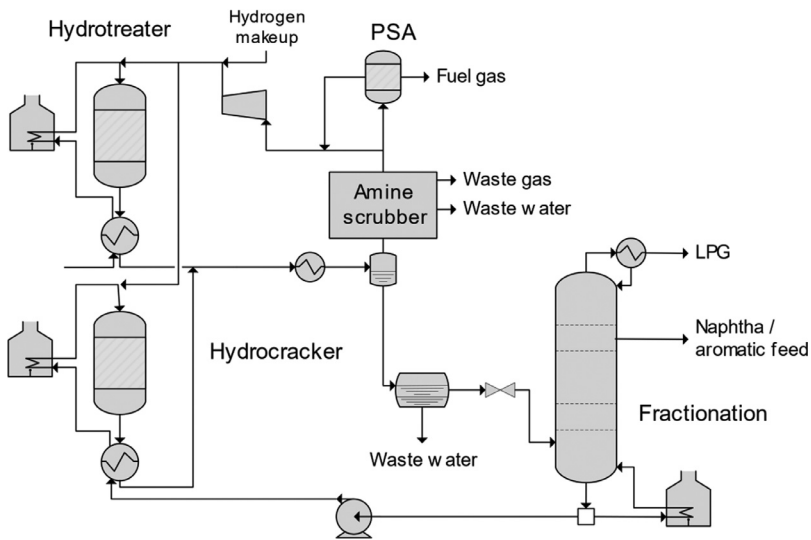


Fig. 19. Visualization of the oil upgrading process.

2.20. Cooling cycle

Multiple processes, especially in the field of gas separation, have a need for low-temperature refrigeration. In practical applications, this is usually represented by the integration of produced gases in compression/release cycles. In this investigation, a representative three-stage refrigeration cycle is assumed and modelled, which associates the refrigeration demand at three temperature levels with the specific electricity and cooling water demand.

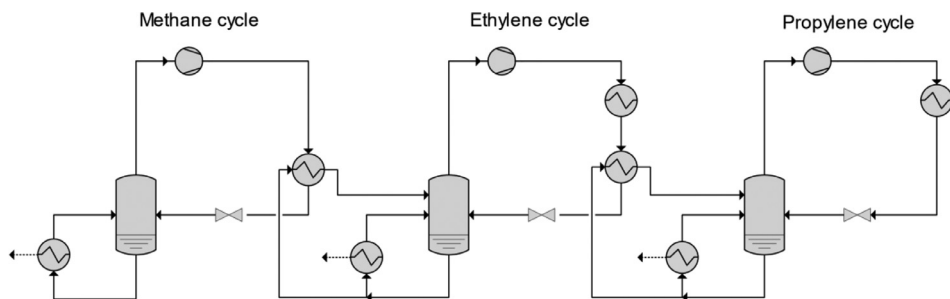


Fig. 20. Visualization of the cooling cycle process.

2.21. Process chain balancing and hydrogen integration

The individual process models are applied for the respective chemical process chain and modelled and balanced in combination to generate coherent mass and energy balances. After process step integration, the following auxiliary process steps are applied.

For gasification and partial oxidation-based processes for production of carbonaceous products (methanol, aromatics, olefins, FT naphtha), external hydrogen can be applied to improve product yield and lower CO₂ emissions [14,15]. Instead of applying the CO shift process to adjust the syngas composition, this is achieved by addition of hydrogen before the synthesis step. For methanol-based synthesis, CO₂ can be maintained in the syngas and converted in the synthesis, as long as the required syngas modulus is achieved. Thus, CO₂ removal by AGR can be avoided, only selective sulfur recovery is required, leading to lowered emissions of concentrated CO₂. For Fischer-Tropsch synthesis on Co-based catalysts, CO₂ is not applicable [16] and is therefore largely removed before the synthesis. Still, the adjustment by CO shift can be substituted to avoid CO₂ formation. Inventories for processes with efficiency increase by hydrogen addition are marked with H.

2.22. Waste gas incineration

Occurring waste gases cannot be emitted directly but must be processed by thermal post-treatment. Flue gas heat is recovered for steam generation. Resulting emissions of CO₂ and SO₂ can be balanced directly from the gas composition. Other ecologically relevant flue gas components follow kinetic formation mechanisms and are therefore approximated by industrial emission values. These values are further applied for fired heating processes.

2.23. Waste water treatment

Wastewater treatment is balanced according to a life cycle inventory model for waste water treatment in the chemical sector [18]. Waste water compositions from Aspen Plus are converted

Table 6

Modelling assumptions of the waste gas incineration process.

Flue gas temperature after energy recovery	200°C
Burner excess air ratio	1.2
Non-fuel specific emission values	[17]
Reference state	Flue gas dry, 3 vol.-% Oxygen
CO	40 mg / m ³ (STP)
Particles	0.5 mg / m ³ (STP)
NOX	100 mg / m ³ (STP)

into defined pollutant parameters. Calculated processing steps include nanofiltration, extraction, wet-air oxidation, mechanical-biological treatment and sludge incineration. The WWT system configuration is adjusted depending on waste water composition to fulfil emission limits, given in [18].

Table 7

Overview waste water treatment balancing components.

Water pollutant parameter	TOC (TOC _{degradable} , TOC _{refractory}), AOX, N _{total} , NH ₄ ⁺ -N, Cl ⁻ , SO ₄ ²⁻
Balanced utilities	Steam, electricity, deionized water, process water, natural gas, caustic soda, sulfuric acid
Balanced emissions to air	Ash, CO ₂ , CO, NO _x , SO ₂ , Dust

2.24. Utility balancing

Utilities are balanced in conclusion over all included process steps. Cumulated process utilities are reported under the following assumptions:

- Produced fuel gas combustion is applied for direct heating and supply of HP and IP steam.
- Excess HP and IP steam is thermally integrated for electricity production.
- Cooling water is applied in a closed cycle with water loss of 2% due to evaporation [19].
- Boiler feed water is prepared by membrane separation processes, adapted from [20] with utility demand per t BFW: 1.175 t Fresh water, 0.66 kWh electricity.

CRediT Author Statement

Florian Keller: Conceptualization, Methodology, Validation, Investigation, Writing - Original Draft, Visualization; **Patricio Mamani Soliz:** Validation, Investigation; **Ludwig Georg Seidl:** Validation, Investigation; **Roh Pin Lee:** Conceptualization, Writing - Review & Editing, Project administration, Funding acquisition; **Bernd Meyer:** Conceptualization, Writing - Review & Editing, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Any opinions, findings, conclusions and recommendations in the document are those of the authors and do not necessarily reflect the view of the BMBF.

Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi:[10.1016/j.dib.2022.107848](https://doi.org/10.1016/j.dib.2022.107848).

References

- [1] R. Reimert, F. Marschner, H.-J. Renner, W. Boll, E. Supp, M. Brejc, W. Liebner, G. Schaub, in: *Gas Production, 2. Processes*, in: *Ullmann's Encyclopedia of Industrial Chemistry*, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2000, p. 38.
- [2] M. Bertau, H. Offermanns, L. Plass, F. Schmidt, H.-J. Wernicke, *Methanol: The basic chemical and energy feedstock of the future*, Springer, Berlin, Heidelberg, 2014.
- [3] M. Gräbner, *Industrial coal gasification technologies covering baseline and high-ash coal*, Wiley-VCH, Weinheim, Germany, 2015.
- [4] M. Gräbner, B. Meyer, Performance and exergy analysis of the current developments in coal gasification technology, *Fuel* 116 (2014) 910–920, doi:[10.1016/j.fuel.2013.02.045](https://doi.org/10.1016/j.fuel.2013.02.045).
- [5] C. Higman, M. van der Burgt, *Gasification*, Elsevier, 2008.
- [6] L. Picard, *Development Status of BGL-Gasification*, Freiberg, 2005.
- [7] D. Chen, L. Yin, H. Wang, P. He, Pyrolysis technologies for municipal solid waste: a review, *Waste Manag.* (2014) 2466–2486, doi:[10.1016/j.wasman.2014.08.004](https://doi.org/10.1016/j.wasman.2014.08.004).
- [8] S.D. Anuar Sharuddin, F. Abnisa, W.M.A. Wan Daud, M.K. Aroua, A review on pyrolysis of plastic wastes, *Energy Convers. Manage.* 115 (2016) 308–326, doi:[10.1016/j.enconman.2016.02.037](https://doi.org/10.1016/j.enconman.2016.02.037).
- [9] S.M. Al-Salem, A. Antelava, A. Constantinou, G. Manos, A. Dutta, A review on thermal and catalytic pyrolysis of plastic solid waste (PSW), *J. Environ. Manage.* (2017) 177–198, doi:[10.1016/j.jenvman.2017.03.084](https://doi.org/10.1016/j.jenvman.2017.03.084).
- [10] C. Haupts, *Wertschöpfung durch CTC-Technologie – nachhaltig, wirtschaftlich, dezentral umsetzbar*, in: E. Thomé-Kozmiensky, O. Holm, B. Friedrich, D. Goldmann (Eds.), *Recycling und Sekundärrohstoffe*, Band 13, Thomé-Kozmiensky Verlag GmbH, Nietwerder, 2020.
- [11] C. Haupts, *Status und Herausforderungen bei der Anwendung des CTC-Verfahrens am Beispiel der Pilotinstallation in Ennigerloh*, Freiberg, 2019.
- [12] C. Vasile, M.A. Brebu, T. Karayıldirim, J. Yanik, H. Darie, Feedstock recycling from plastics and thermosets fractions of used computers. II. Pyrolysis oil upgrading, *Fuel* 86 (2007) 477–485, doi:[10.1016/j.fuel.2006.08.010](https://doi.org/10.1016/j.fuel.2006.08.010).
- [13] P. Kokayeff, S. Zink, P. Roxas, *Hydrotreating in Petroleum Processing*, in: S.A. Treese, D.S. Jones, P.R. Pujado (Eds.), *Handbook of Petroleum Processing*, Springer International Publishing, Cham, 2015, pp. 1–59.
- [14] L.G. Seidl, W.-R. Poganietz, F. Keller, R.P. Lee, A. Grunwald, B. Meyer, *Konzepte und Nachhaltigkeitsbewertung der Kohlenstoffkreislaufwirtschaft am Beispiel des chemischen Recyclings zur Olefinproduktion*, *Chem. Ing. Tech.* 244 (2020) 118629, doi:[10.1002/cite.202000102](https://doi.org/10.1002/cite.202000102).
- [15] M. Ostadi, K.G. Paso, S. Rodriguez-Fabia, L.E. Øi, F. Manenti, M. Hillestad, *Process Integration of Green Hydrogen: Decarbonization of Chemical Industries*, *Energies* 13 (2020) 4859, doi:[10.3390/en13184859](https://doi.org/10.3390/en13184859).
- [16] M.E. Dry, *FT catalysts*, in: *Fischer-Tropsch Technology*, Elsevier (2004) 533–600.
- [17] B. Pascal, M. Chaugny, L. Delgado Sancho, S. Roudier, *Best available techniques (BAT) reference document for the refining of mineral oil and gas industrial emissions: Industrial Emissions Directive 2010/75/EU (integrated pollution prevention and control)*, Publications Office, Luxembourg, 2015.
- [18] A. Köhler, S. Hellweg, E. Recan, K. Hungerbühler, *Input-dependent life-cycle inventory model of industrial wastewater-treatment processes in the chemical sector*, *Environ. Sci. Technol.* 41 (2007) 5515–5522, doi:[10.1021/es0617284](https://doi.org/10.1021/es0617284).
- [19] U. Vengateson, *Cooling towers: estimate evaporation loss and makeup water requirements*, 2017. https://www.chemengonline.com/cooling-towers-estimate-evaporation-loss-and-makeup-water-requirements/#disqus_thread (accessed 15.01.21).
- [20] C. Ras, H. von Blottnitz, *A comparative life cycle assessment of process water treatment technologies at the Secunda industrial complex, South Africa*, *WSA* 38 (2012), doi:[10.4314/wsa.v38i4.10](https://doi.org/10.4314/wsa.v38i4.10).