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Sustainable aviation fuel from Kraft lignin – Technical, economic and ecological process analysis

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ABSTRACT

Molten salt supported catalytic depolymerisation of lignin is an attractive option for the production of sustainable aviation fuel, exploring lignin's high content of aromatic hydrocarbons. The European project 'ABC-Salt' developed a concept involving in-situ hydropyrolysis in salts and catalytic hydrodeoxygenation to obtain middle distillates from Kraft pulp mill lignin. This study evaluates the technical, economic and ecological viability of the proposed power-and-biomass-to-liquid process and its integration into the lignin providing pulp mill via a comprehensive techno-economic assessment (TEA) and life cycle assessment (LCA). The process analysis indicates a very high carbon efficiency of 78 % and an energy efficiency of 52.5 $\%_{LHV}$. The net production cost amounts to 1.66 $€_{2020}/l_{Fuel}$ with lignin as the highest cost contributor. Lignin is also the biggest contributor to a majority of environmental impacts, which increases the importance of the selected allocation method for lignin extraction at the pulp mill. In dependence of the allocation method, global warming potential savings range between 72 and 89 %, while major impact increases compared to fossil jet fuel occur in categories like water use, land use, minerals and metals resource depletion or freshwater eutrophication. Since hydrogen is essential for deoxygenation of the fuel, recovery of unused hydrogen is a key parameter for TEA and LCA results. The lowest cost and environmental impacts can be found for hydrogen recovery rates between 95 and 98 %. Finally, based on both TEA and LCA, currently a CO_2 price of around 500 $€/t_{CO_2\text{-eq.}}$ would be necessary in order to produce cost competitive jet fuel.

1. Introduction

The European Union has a strong commitment to mitigate climate change, aiming to reduce greenhouse gas (GHG) emissions by 55 % in 2030 in comparison with those of 1990 and becoming climate neutral by 2050 (European Commission, 2021). For the transport sector, the European Parliament set the target to reach at least 29 % renewables within the final energy consumption by 2030 (European Parliament, 2023). Novel processes must be developed to diversify the energy supply and the dependence on fossil fuels in transport. Waste streams appear to be excellent feedstock candidates for new fuels as they overcome feedstock limitations, enhancing the cost-effectiveness and sustainability of processes using them.

The European HORIZON 2020 project 'ABC-Salt' provides innovative technical solutions and a holistic approach for the production of middle distillate range biofuels from lignocellulosic wastes through an advanced thermochemical conversion power-and-biomass-to-liquid process (PBtL). Considering biogenic carbon as the core element for transportation fuels, lignocellulosic biomass waste streams are aimed at as a feedstock. In particular, lignin, which accounts for ~25–30 % of carbon in lignocellulosic biomass and consists of nearly 50 % aromatic hydrocarbons, is an attractive candidate for fuel production although depolymerisation is a challenging task due to its high natural complexity (Xu et al., 2014). As a side product of the pulp and paper industry, lignin is generally chemically underutilised and limited to energetic use by combustion for heat and power purposes (Xu et al., 2014). The Kraft (or sulphate) pulping process is hereby the by far most common method

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Nomenclature

AEL	Alkaline electrolysis
ABC-Salt	Advanced Biomass Catalytic Conversion to Middle Distillates in Molten Salts
CH	Switzerland
ETS	Emission trading system
FCI	Fixed capital investment
GHG	Greenhouse gas
GLO	Global
GWP	Global warming potential
HEX	Heat exchanger
HP	Hydropyrolysis
HDO	Hydrodeoxygenation
IAI Area, EU27 & EFTA	Aluminium industry specific electricity market for aluminium-producing countries within EU27 and EFTA (European Free Trade Association)
IH2	Integrated hydro pyrolysis plus hydro conversion
LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
LHV	Lower heating value
MFSP	Minimum fuel selling price
PBtL	Power-and-biomass-to-liquid
RED II	Renewable Energy Directive II
RER	Europe
RISE	Research Institute of Sweden
SAF	Sustainable aviation fuel
SE	Sweden
TEA	Techno-economic assessment
TEPET	Techno-economic process evaluation tool

Variables (greek characters)

η_C	Carbon efficiency [%]
η_{energy}	Energy efficiency [%]

Variables (latin characters)

ACC	Annuity [€/a]
B_j	Basis for cost factor j [€/a, €]
c_{labour}	Labour costs [€/h]
$C_{R\&B\&U,i}$	Market price for raw material, by-product or utility i [€/kg, €/m^3, €/MWh, …]
$CEPCI$	Chemical engineering plant cost index [-]
CPI	Commodity price index [-]
d_i	Dimensiong factor for equipment scaling [-]
EC_i	Equipment cost of equipment i [€, \$]
$EC_{Ref,i}$	Equipment cost of reference equipment i [€, \$]
FCI	Fixed capital investment [€]
$F_{eco,i,j}$	Capital cost factor j for equipment i [-]
$F_{ecoII,j}$	Operational cost factor j [-, a^{-1}]
h_{labour}	Labour hours [h/a]
IR	Interest rate [%]
LHV_{fuel}	Lower heating value of fuel [MJ/kg]
$LHV_{lignin,dry}$	Lower heating value of dry lignin [MJ/kg]
$\dot{m}_{C,fuel}$	Carbon mass flow in fuel [kg/h]
$\dot{m}_{C,lignin,dry}$	Carbon mass flow in dry lignin [kg/h]
$\dot{m}_{fuel/lignin,dry}$	Mass flow of fuel or dry lignin [kg/h, kg/a]
m_i	Quantity of stream i [kg/a, m^3/a, MWh/a, …]
N	Plant operating time [a]
NPC	Net production costs [€/kg, €/MJ]
$OPEX_{direct,i}$	Direct operational expenditure i [€/a]
$OPEX_{indirect,j}$	Indirect operational expenditure i [€/a]
P_{el}	Process electricity consumption [MW]
S_i	Capacity of equipment i [t/h, MW, m^3/h, m^2, …]
$S_{Ref,i}$	Capacity of reference equipment i [t/h, MW, m^3/h, m^2, …]
TPC	Total production costs [€/a]
x_{WC}	Working capital share [%]

used for pulp production and provides Kraft lignin with its characteristic name (Argyropoulos et al., 2023).

Considering Kraft lignin as a widely available feedstock for future sustainable aviation fuel (SAF) production, a new concept is proposed. The concept involves in-situ hydropyrolysis in salts and catalytic hydrodeoxygenation, which essentially combines all beneficial aspects of existing technologies (fast pyrolysis, hydrothermal liquefaction, integrated hydro pyrolysis plus hydro conversion (IH2) technology and existing molten salt systems). A major issue of alternatives, and specifically the catalytic hydropyrolysis as in IH2, is the feeding of solid biomass to a pressurized reactor (Marker et al., 2011). In ABC-Salt this is effectively eliminated by using a solubilised biomass source in a suitable medium. In addition, for conventional pyrolysis of solid biomass, rapid heating of the biomass particles is required to optimize the vapour yield and to minimize char and gas formation (Bridgewater, 2004). This requires small biomass particles and the use of an inert heat carrier (sand) (Bhaskar et al., 2011), which is not required in this concept. As such, the use of a solubilised biomass source in combination with an excellent heat carrier (molten salt) may lead to higher biomass to hydrocarbon yields than existing processes.

Several techno-economic assessments (TEA) and life cycle assessments (LCA) are available in literature for lignocellulosic biomass to fuel conversion via fast pyrolysis with subsequent hydrotreating or IH2. Jones et al. (2013), for example, investigated the former pathway for the production of gasoline equivalent fuel from woody feedstocks (\$ 80/t_{dry}). The authors indicated a minimum fuel selling price (MFSP) of $\$_{2011}$ 0.91/$l_{gasoline}$ and global warming potential (GWP) in the range of 28–39 $g_{CO2\text{-}eq.}/MJ_{gasoline}$. A newer study by Ma et al. (2024) calculated levelized fuel production cost of around $\$_{2022}$ 0.69–0.76/$l_{biofuel}$ and a GWP between 19.3 and 52.4 $g_{CO2\text{-}eq.}/MJ_{biofuel}$ with miscanthus (\$ 33/t) as feedstock. The IH2 process, on the other hand, indicates a MFSP of $\$_{2007}$ 0.43/$l_{gasoline}$ (Tan et al., 2013) and GWP of 10.4 $g_{CO2\text{-}eq.}/MJ_{gasoline}$ (Zupko, 2019) with wood (\$ 72/$t_{US,dry}$) or, in the case of GWP, woody residues as feedstock. Further environmental impacts considered were fossil energy consumption in the case of fast pyrolysis with subsequent hydrotreatment (Jones et al., 2013; Ma et al., 2024) and ozone depletion, smog, acidification, eutrophication, carcinogenics, non-carcinogenics, and respiratory effects in the case of IH2 (Zupko, 2019).

TEAs and LCAs of hydrocarbon fuels with lignin as feedstock are, however, scarce. Especially, when lignin valorisation is not just implemented as a credit to the technical, economic and ecological results of the main product. Three publications were found in which the individual cost and GWP of biofuel produced from lignin were analysed. The first biofuel production process involves pretreatment followed by hydrodeoxygenation and estimates a MFSP price of $\$_{2014}$ 0.95/$l_{jet\text{-}fuel}$ (Shen et al., 2018). The second one comprises fast pyrolysis with subsequent hydrotreatment and -cracking, which yields production cost of around $\$_{2014}$ 0.50–0.75/$l_{biofuel}$ and a GWP in the range of 51.5–151.1 $g_{CO2\text{-}eq.}/MJ_{biofuel}$ (Obydenkova et al., 2017). Both of the formerly mentioned studies used lignin waste from ethanol plants as an input. The third publication investigates biofuel production from pulp mill lignin or black liquor through lignin liquefaction and hydrotreatment or black liquor gasification and methanol to fuel synthesis. Depending on the biofuel process and pulp mill configuration, MFSPs between 77 and 150 €$_{2017}$/$MWh_{biofuel}$ and GWPs from −33 to 29 $g_{CO2\text{-}eq.}/MJ_{biofuel,\ LHV}$ were determined (Jafri et al., 2020). The GWP was calculated with a simplified approach grounded in the Renewable Energy Directive II (RED II) method with substitution for the natural gas by-product.

The objectives of this study are to quantify cost and environmental impacts associated with SAF produced from Kraft lignin via the pulp mill integrated ABC-Salt process and validate the novel process concept as a viable biofuel pathway in alignment with EU's climate change mitigation targets. In comparison to a standard catalytic hydropyrolysis, the ABC-Salt process has two notable novelties, namely the use of molten salt as a catalyst in the hydropyrolysis and the recycling of partial amounts of hydrodeoxygenation product as liquefaction agent for the hydropyrolysis. As stated before, this improves the feeding of lignin to the pressurized units and ensures good heat transfer, which in turn reduces char formation. The techno-economic and life cycle assessment are conducted based on standardised methodology previously published in literature by Peters et al. (2003) and ISO 14040/14044 (ISO 14040, 2006; ISO 14044, 2017), respectively. As both process steps, hydropyrolysis and hydrodeoxygenation, use H_2 for oxygen reduction, H_2 consumption is a key aspect. Its use puts a strain on the economic-ecological sustainability when overconsumed, but also ensures an efficient enough carbon conversion and therefore an improved fuel yield. Hence, recovery rates of unreacted H_2 are investigated in more detail in a sensitivity analysis.

2. Methodology

The ABC-Salt process consists of a hydropyrolysis (HP) unit, two subsequent hydrodeoxygenation (HDO) units, a membrane unit for hydrogen recovery, and a water electrolyser (see 2.2 for the detailed process description). In addition, the ABC-Salt process is integrated with a pulp mill, allowing material and energy exchange (Fig. 1). Gaseous by-products (the hydrogen depleted stream from the membrane unit), char and excess heat/steam is transferred to the pulp mill for electricity generation. In return, the pulp mill provides the ABC-Salt process with electricity and dried lignin (8 $\%_{wt.}$ moisture content). Apart from the exchanged streams and mentioned valuable products, the pulp mill is fed with pulp wood and chemicals (CO_2, H_2SO_4, H_2O_2, $MgSO_4$, NaOH, O_2, SO_2, CH_3OH, $NaClO_3$, CaO) and produces some waste in form of gases (biogenic CO_2, SO_2), liquids (wastewater) and solids (recovery boiler dust, bark boiler ash, biosludge, green liquor dregs, lime mud, slaker grits). The main products from the ABC-Salt process are the desired middle distillates, also referred to as sustainable aviation fuel (SAF), and an aqueous phase that contains the salt and (limited amounts of) dissolved hydrocarbons. Further inputs to the ABC-Salt process comprise salt, hydrochloric acid for washing of the HP product to remove salt, and electrolyte solution for hydrogen production through electrolysis.

2.1. Experiments and unit models

Reaction equations for the process model were set up based on data from the experiments, which are shortly described hereinafter, and model compounds were selected accordingly.

2.1.1. Experimental description and product analysis

Experimental data for the ABC-Salt process model development was consolidated from long-term experiments (100 h). A schematic depiction of the experimental ABC-Salt process set-up can be found in SI-Fig. 1.1. The process involved the dissolution of softwood based Kraft lignin in simple phenols at a mass ratio of 1:3 with 2.5 $\%_{wt.}$ molten salts (based on lignin input with 8 % moisture) acting as a catalyst. The molten salt catalyst used was a mixture of $ZnCl_2$, KCl and NaCl (ratio: 44.3, 41.9 and 13.8 $\%_{mol}$, resp.). The dissolved feed solution (lignin, simple phenols and salts) was pumped into a pressured autoclave reactor (100 ml Parr autoclave) at 330 °C and 100 bar. The added salt is removed from the thereby obtained HP oil by a dilute acid wash and the cleaned oil is converted to the desired final hydrocarbon rich liquids by a two-step catalytic HDO with pre-sulfided $NiMo/Al_2O_3$ as catalyst in a packed bed reactor. The simple phenols, along with the other lignin derived monomers, are removed after the first catalytic HDO step and the former are reused as diluent for HP. The final hydrotreated product was distilled into three fractions based on boiling temperature: a light fraction ($T < 110$ °C, 22 $\%_{wt.}$), a middle distillate fraction ($110 < T < 260$ °C, 73 $\%_{wt}$) and a residue ($T > 260$ °C, 5 $\%_{wt}$).

The composition of the middle distillate fraction was measured using 2D GC- FID analysis (see SI-Fig. 1.4 for chromatogram). The quantitative concentrations of identified product groups are listed in Table 1. Three major product groups are visible: cycloalkanes, straight chain alkanes and aromatic hydrocarbons (aromatics). Cycloalkanes account for nearly half of the hydrotreated product, composed majorly of substituted cyclohexanes and cyclopentanes. Straight chain alkanes and aromatics make up the rest of the product. Hardly any oxygenated phenolic groups such as cresols and guaiacols were measured after the second hydrodeoxygenation step.

2.1.2. Selection of model compounds and model development

The compounds listed in Table 2 are chosen as representatives for the process simulation. A compound with the molecular formula of $C_{20}H_{24}O_6$ was chosen as the nearest Kraft lignin representative with a comparable stoichiometry and defined properties in the Aspen Plus® V10 database. The depolymerized oil after HP was represented as a 4,4-dimethoxystillbene. During the first (milder) HDO step noticeable

Table 1
Mass fractions of different product groups in the final deoxygenated product determined by 2D GC-FID analysis.

Product group	Mass fraction [$\%_{wt.}$]
Cycloalkanes	56.92
Straight chain alkanes	20.28
Aromatics	21.51
Naphthalenes	0.00
Ketones	0.01
Volatile Fatty Acid	1.23
Methoxyphenolics	0.02
Phenols	0.01
Dihydroxybenzenes	0.02

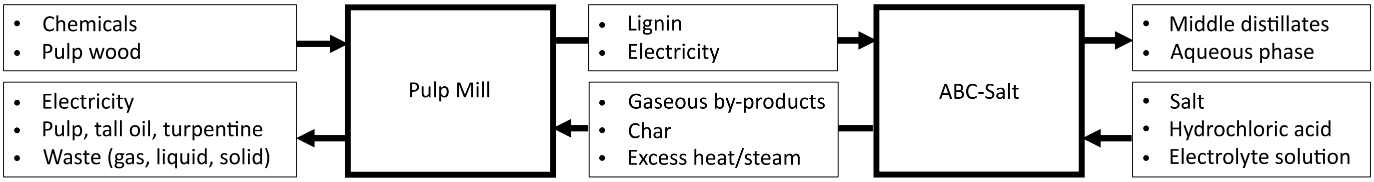

Fig. 1. Block flow diagram of the main streams entering the ABC-Salt and pulp mill process and the streams that are exchanged between the two processes.

Table 2
Suggested model compounds for the flow sheeting.

Main components	Location in flowsheet	Model compound		Chemical Formula
LignoBoost lignin	HP_{in}			$C_{20}H_{24}O_6$
HP oil	HP_{out}		4,4-Dimethoxystilbene	$C_{16}H_{16}O_2$
Diluent for HP	$HDO\text{-}1_{out}$		m-Cresol	C_7H_8O
Stabilised HP oil	$HDO\text{-}1_{out}$		8-phenylmenthol	$C_{16}H_{24}O$
Final hydrotreated product	$HDO\text{-}2_{out}$	Cycloalkanes	Cyclohexane	C_6H_{12}
			Ethyl Cyclopentane	C_7H_{14}
			Ethyl Cyclohexane	C_8H_{16}
			Propyl Cyclohexane	C_9H_{18}
			Cyclohexane, 1,1'-(1,2-ethanediyl)bis-	$C_{14}H_{26}$
		Aromatics	O-Xylene	C_8H_{10}
			P-Xylene	C_8H_{10}
			M-Xylene	C_8H_{10}
Char	HP_{out}		Non-Conventional solid	C: 75.33 $\%_{wt.}$ H: 6.30 $\%_{wt.}$ O: 18.37 $\%_{wt.}$

hydrogenation occurs, hence the stabilised HP oil model compound is assumed to be hydrogenated to 8-Phenylmenthol, which is chosen based on a similar elemental composition compared to experimental results. Additionally, some of the HP oil is hydrocracked, mostly to simple phenols (represented by m-Cresol) and methane. Products after the second HDO step fall broadly into two product groups, cycloalkanes and aromatics (see Table 1). Straight chain alkanes are grouped here together with the cycloalkanes due to their very similar stoichiometry. Five cycloalkanes with different numbers of carbon atoms were chosen as the representative cycloalkanes and isomers of xylene were chosen as the representative aromatic compounds since they were the most abundant compounds found in the hydrotreated product. The chemical reaction equations used in the different steps of the process simulation are listed in Table 3, which also include the gases measured during experiments. The stoichiometric reactions were established by selecting their conversion and stoichiometric coefficients to fit the experimentally measured data.

2.2. ABC-salt process model description and assumptions

The process model depicted in Fig. 2, including the main conditions in the various units, is set up in Aspen Plus® V10 using the Peng Robinson equation of state with the Boston-Mathias alpha function (PR-BM). Char is introduced as a non-conventional component with proximate and ultimate analysis data based on mass balance calculations (SI-Table 2.1). Its enthalpy is determined with the implemented property method for coal HCOALGEN, which utilises the proximate, ultimate and sulphur analysis data. The reaction equations for HP and HDO-1/-2 are derived from experimental work as explained in the previous subchapter. The other process units are modelled based on literature data. The process is scaled according to the lignin input ($3.25\ t_{dry}/h = 3.53$ t/h with 8 $\%_{wt.}$ moisture content) that can be provided by the pulp mill. A detailed summary of the resulting mass flows is available in SI-Table 2.2.

2.2.1. Liquefaction and hydropyrolysis

In a first step lignin enters a centrifugal pump (P-1) together with the salt (see Chapter 2.1.1) and a liquid stream that is separated after HDO-1. The amount of the liquid recycle stream, mainly consisting of simple phenols, is regulated in order to fulfil: $mass_{simple\ phenols} = 3 \cdot mass_{lignin}$. Simple phenols act as a liquefaction agent to provide a pumpable slurry and to ensure excellent heat transfer in the HP. HP is performed at an elevated pressure of 30 bar and temperature of 340 °C in an autoclave, which is modelled with Equation (2.1) in an 'RStoic' reactor. Mixing lignin with simple phenols and salt showed the highest yields in the HP, as very low char yields were seen.

2.2.2. Intermediate cleaning

The HP product is separated in two fractions in a 'Flash2' separator (F-1, 10 bar and 50 °C). While the gaseous fraction continues to a H_2 recovery membrane unit (H_2 RMU) to recover unreacted hydrogen, the bottom fraction of the HP product is further processed by an acidic water washing ($mass_{acidic\ water} = 0.5 \cdot mass_{oil}$, acidic water: 0.05 mol_{HCl}/l). The acidic water is essential to remove the salt from the HP oil. Oil and water phase incl. char are separated in the subsequent hydrocyclone (HC). The

Table 3
Reaction equations for HP, HDO-1 and HDO-2.

Process unit & conversion	Reaction equation	
HP 100 % conversion	$C_{20}H_{24}O_6 + 2.37\ H_2 \rightarrow$ $1.19\ C_{16}H_{16}O_2 + 0.74\ CH_4 + 3.33\ H_2O + 0.14\ CO_2 + \text{Char}$	(2.1)
HDO-1 Hydrogenation of HP oil 92 % conversion	$C_{16}H_{16}O_2 + 5\ H_2 \rightarrow C_{16}H_{24}O + H_2O$	(2.2)
HDO-1 Hydrocracking of HP oil 8 % conversion	$C_{16}H_{16}O_2 + 15\ H_2 \rightarrow C_7H_8O + 9\ CH_4 + 0.01\ CO + H_2O$	(2.3)
HDO-2 Hydrotreatment of stabilised HP oil to aromatics 25 % conversion	$C_{16}H_{24}O \rightarrow \text{O-Xylene} + 0.5\ \text{P-Xylene} + 0.5\ \text{M-Xylene} + H_2O + H_2$	(2.4)
HDO-2 Hydrotreatment of stabilised HP oil to cycloalkanes 75 % conversion	$C_{16}H_{24}O + 5.1\ H_2 \rightarrow$ $0.28\ C_6H_{12} + 0.46\ C_7H_{14} + 1.13\ C_8H_{16} + 0.14\ C_9H_{18} +$ $0.04\ C_{14}H_{26} + 0.02\ C_3H_8 + 0.01\ C_2H_6 + 0.11\ CH_4 + 0.01\ CO + H_2O$	(2.5)
HDO-2 Hydrogenation of excess simple phenols 100 % conversion	$C_7H_8O + 4\ H_2 \rightarrow C_7H_{14} + H_2O$	(2.6)

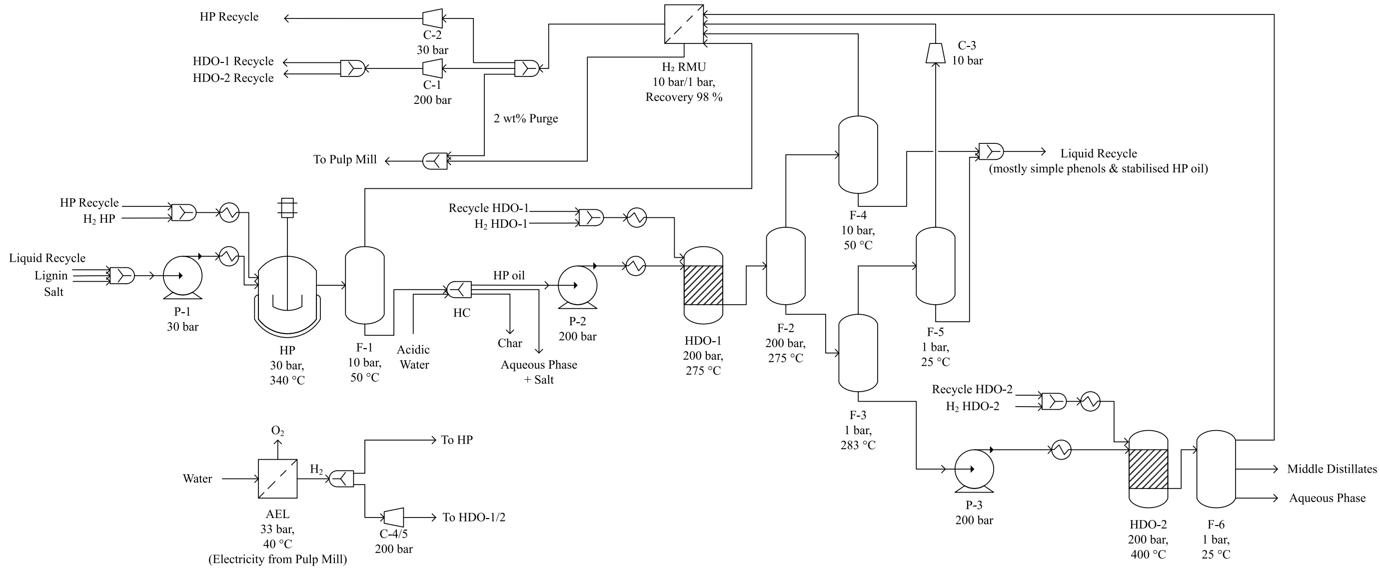

Fig. 2. Aspen Plus® process model of the ABC-Salt process.

HC is modelled as a 'Decanter' with two additional 'Sep' separators, all operating at 1 bar and 30 °C. The two separators are required in the simulation to ensure a defined salt removal of 99.6 % and ideal separation of char from the aqueous solution.

2.2.3. *Hydrodeoxygenation*

Only the HP oil is fed to the milder stabilisation HDO-1 unit, a fixed bed reactor at 200 bar and 275 °C, which is modelled as an 'RStoic' reactor with Equations (2.2) and (2.3). The HDO-1 product is separated in several 'Flash2' separators (F-2 to F-5) targeting the separation into three streams – one consisting mainly of gaseous components that are fed to the membrane unit for hydrogen recovery, one consisting of mainly simple phenols that is recycled to the feed of the centrifugal pump and one fraction that contains the target product which continues to the harsher deep HDO-2, a fixed bed reactor at 400 °C. In HDO-2 the three Reactions (2.4), (2.5) and (2.6) occur, which are modelled with an 'RStoic' reactor. The HDO-2 product is then separated with another 'Flash3' separator (F-6) into three fractions: a gaseous fraction, an aqueous fraction and the target product fraction (middle distillates). Again, the gaseous fraction, consisting of reaction products and unreacted hydrogen, is transferred to the membrane unit for hydrogen recovery. The operating conditions of F-3 are regulated in order to provide the required amount of simple phenols in the liquid recycle for a sufficient phenols-to-lignin feed ratio.

2.2.4. *Hydrogen recovery*

The main assumptions for the H_2 recovery membrane unit (H_2 RMU) are: 98 % hydrogen recovery rate, pressure ratio of 10 bar feed to 1 bar permeate, selectivity of hydrogen to the different components ($H_2/CO_2 = 3.4$, $H_2/CH_4 = 70.4$, $H_2/H_2O = 2$, $H_2/C_2H_6 = 100$, $H_2/CO = 38.5$) and H_2 permeability ($Perm_{H2} = 3.569$ mol m^{-2} h^{-1} bar^{-1}) based on (Zarca et al., 2018; Baker, 2012). From these assumptions the split ratio to permeate and retentate is calculated and modelled in a 'Sep' separator. The calculation of the membrane area, which is required for the cost calculations and LCA, assumes that the selectivity does not affect the area. The membrane area is hence calculated from the pressures, permeate flux, permeability and the molar fractions (SI-Code 2.1). The permeate from the membrane unit is recycled to the process while the retentate continues to the pulp mill for electricity generation. To avoid accumulation of inert gases, 2 $\%_{wt.}$ of the permeate is assumed to be purged. This purge gas also continues to the pulp mill. The remaining permeate is split between the different units approximately according to their total hydrogen demand: 0.2, 0.3, and 0.5 for HP, HDO-1, and HDO-2, respectively. The remaining hydrogen demand is satisfied and regulated by the pure hydrogen produced through water electrolysis.

2.2.5. *Electrolysis*

Hydrogen (100 % purity assumed) is produced in an alkaline water electrolysis (AEL) with a system efficiency of 53.9 kWh/kg_{H2} or 61.8 $\%_{LHV}$ (Kuckshinrichs et al., 2017). The electrolyser requires 10.11 $kg_{deionised\ water}/kg_{H2}$ and 0.275 g_{KOH}/kg_{H2} (Kuckshinrichs et al., 2017). Electricity is provided by the pulp mill (see Chapter 2 preface). Before adding the hydrogen to the two HDO reactors, hydrogen is further compressed to 200 bar with a 'MCompr' compressor while the hydrogen for the HP reactor is kept at the outlet pressure of 33 bar. The total amount of hydrogen fed to the reactors is based on the experimental work: 6 g H_2/100 g lignin, 10 g H_2/100 g lignin and 19 g H_2/100 g lignin for HP, HDO-1 and HDO-2, respectively.

2.2.6. *Liquid recycle*

Liquid is recycled from F-4 and F-5 to the beginning of the process in order to liquify the otherwise solid lignin and salt streams. As explained previously simple phenols are used as the liquefaction agent for HP, which requires 10.6 t/h of simple phenols to be recycled for the 3.53 t/h of lignin input. However, simple phenols are only produced in the HDO-1 reactor (2.3), resulting in 92.8 $kg_{simple\ phenols}/h$. A very high recovery rate >99 % of simple phenols is therefore needed which entails rather sophisticated processing and leads to an accumulation of the stabilised HP oil in particular. As a result, a high liquid recycling rate of 34 t/h (31 $\%_{wt.}$ simple phenols, 68 $\%_{wt.}$ stabilised HP oil) is observed to process 3.53 t/h of lignin. This large throughput has an impact on the sizing of the equipment and, hence, the net production cost. The remaining simple phenols end up either in the final product (73 %), gas (6 %) or aqueous phase (21 %).

2.3. *Pulp mill process model description and assumptions*

RISE's reference mill model represents a theoretical softwood Kraft pulp mill that was used for estimation of lignin production and integration with the ABC-Salt process. The steady-state model, built in the process simulation software WinGEMS (Valmet™), contains complete mass and energy balances of the entire mill, including all relevant unit operations of a pulp mill. The model features some custom developed blocks, chemical equilibrium reactions as well as pulp mill process chemistry knowledge gained from years of internal research projects. In this work, the pulp mill production capacity was fixed to an annual production of 700000 ton air dried pulp (i.e. 90 % dry content). A more detailed schematic diagram and description of the reference model can be found in SI-Chapter 3. The pulp mill model also features the option to extract lignin from the black liquor via the LignoBoost concept (owned by Valmet™). The amount of lignin produced by the LignoBoost process is around 26000 $t_{lignin,dry}/a$ or 3.25 $t_{lignin,dry}/h$ with an analytically determined lower heating value of 26 $MJ_{LHV}/kg_{lignin,dry}$. This corresponds to a separation of around 7 % of the original lignin available in the black liquor.

The side products from the ABC-Salt process are integrated into the pulp mill process as follows (SI-Figure 3.3): The gaseous by-products (700 kg/h, 42.6 MJ_{LHV}/kg) are combusted in the recovery boiler as the recovery boiler already has specific burners for combustion of non-condensable gases. The char (9 kg/h, 30.5 MJ_{LHV}/kg) is combusted in the pulp mill's external biomass boiler due to its dry content and to avoid unnecessary accumulation of non-process related elements in the pulp mill (originating from the salt). The excess steam (5.9 t/h, 10 bar, 180 °C) is mixed directly into the pulp mill's middle pressure headers for internal consumption. That way, less steam needs to be tapped off from the high-pressure headers for internal use and the power production can be maximised. 4.4 MW power can be produced from the side products and around 18.8 MW of the pulp mill excess power (83.4 MW) are in turn delivered to the ABC-Salt process.

A few assumptions were made in the model for lignin production as well as for the integration with the ABC-Salt process:

- The lignin yield (~250 $kg_{lignin}/t_{black\ liquor,\ dry\ solids}$), consumption of CO_2 (200 $kg/t_{lignin,dry}$) and H_2SO_4 (180 $kg/t_{lignin,dry}$), and the remaining ash composition in the lignin are based on average values from various lignin separation experiments conducted at RISE throughout the years.
- The pulp mill does not increase its production of pulp when separating lignin, even though lignin separation is often used as an argument for pulp mills to unload the recovery boiler in order to increase the pulp production, which is usually the bottleneck.
- The Na/S balance at the pulp mill is maintained constant during the lignin separation, i.e. any changes in the Na/S balance are counteracted with necessary recovery boiler dust purging and addition of makeup chemicals.
- There is an overcapacity in the pulp mill's biomass and recovery boilers to handle the addition of char and gaseous by-products, respectively.

2.4. Technical assessment

The energy efficiency η_{energy} expresses the share of energy transferred to the middle distillate product (fuel) from the one entering the process in chemical or electrical form:

$$\eta_{energy} = \frac{\dot{m}_{fuel} \times LHV_{fuel}}{P_{el} + \dot{m}_{lignin,dry} \times LHV_{lignin,dry}} \tag{2.7}$$

where $\dot{m}_{fuel}$ and $\dot{m}_{lignin,dry}$ represent the mass flows of produced fuel and dry lignin input, respectively. LHV_{fuel} and $LHV_{lignin,dry}$ are the lower heating values of fuel and dry lignin. P_{el} stands for any additional electricity consumption of the process.

The carbon efficiency η_C is defined as the amount of carbon from dry lignin that ends up in the fuel:

$$\eta_C = \frac{\dot{m}_{C,fuel}}{\dot{m}_{C,lignin,dry}} \tag{2.8}$$

where $\dot{m}_{C,fuel}$ and $\dot{m}_{C,lignin,dry}$ are the mass flows of carbon in the fuel and dry lignin, respectively.

Table 4
General plant assumptions.

Plant capacity	3.53 t/h lignin (8 % moisture)
Full load hours	8000 h
Plant operating time	25 years
Interest rate	7 %
Base year	2020
Location	Sweden, brownfield

2.5. Economic assessment

The underlying methodology for basic cost estimation of the net production cost (NPC) is provided by Peters et al. (2003), which is intended to provide a decision basis for the implementation of a detailed design. Basic plant assumptions are shown in Table 4 and are the same for both processes, the ABC-Salt and pulp mill process.

The *NPC* is calculated from the annuity (*ACC*), direct and indirect operational expenditure (*OPEX*), labour hours (h_{labour}) and costs (c_{labour}) and the resulting fuel or lignin production amount $\dot{m}_{fuel/lignin}$:

$$NPC = \frac{ACC + \sum_{i}^{m} OPEX_{direct,i} + \sum_{j}^{10} OPEX_{indirect,j} + h_{labour} \times c_{labour}}{\dot{m}_{fuel/lignin,dry}} \tag{2.9}$$

The remaining equations for annuity and operational expenditures are listed in Appendix A.1.

2.5.1. ABC-salt process

The net production cost of the ABC-Salt middle distillates is calculated by coupling the Aspen Plus® simulation with DLR's 'techno-economic process evaluation tool' TEPET (Albrecht et al., 2017), which automated the above mentioned methodology. Stream data are transferred to TEPET for estimating the equipment costs and costs for raw materials and utilities. The underlying assumptions for the purchased equipment cost EC_i are listed in Table A.1 and the capital cost factors $F_{eco,i,j}$ to obtain the fixed capital investment can be found in SI-Table 4.2. The working capital share (x_{WC}) is set to 10 % for the ABC-Salt process. Operational cost factors $F_{ecoII,j}$ and their basis B_j are defined in the right column of SI-Table 4.1 for indirect OPEX. Labour hours are estimated with 32339.5 h/a according to Peters et al. (2003) for average conditions, a product output of 1974.39 kg/h, and 5 production steps. The labour costs for 2020 are determined using labour cost indices (2020: 108.1, 2016: 99.6) (Statistisches Bundesamt, 2022) and labour costs of 49.96 $€_{2016}/h$ (Eurostat, 2020) in Sweden. The assumed market prices for all considered raw materials and utilities can be found in Table A.2. Moreover, replacement cost for the hydrogen recovery membrane and AEL stack are included there as well. The lignin cost is derived from the pulp mill integration studies (see Chapter 2.5.2 and 3.2).

2.5.2. Pulp mill process

The production cost of lignin is considered to be the additional operational and capital cost compared to no lignin extraction at all, i.e., only pulp production. Specific prices of consumables as well as the purchased equipment cost associated with a complete LignoBoost plant (that includes all equipment and installation work) are shown in Table A.3. The only additional cost factor included for the fixed capital investment is contingency with 20 %. Indirect OPEX comprises maintenance with an operational cost factor $F_{ecoII,j}$ of 0.03 and fixed capital investment as the basis (B_j). Working capital share x_{WC} as well as additional labour costs are set to 0.

2.6. Ecological assessment

The life cycle assessment (LCA) for the ABC-Salt middle distillates is performed, like the economic assessment, based on the Aspen Plus® simulation in combination with DLR's TEPET extension (Weyand et al., 2023). The latter is built upon the open source LCA software framework Brightway2 (Mutel, 2017). All stream data are coupled with background data from the ecoinvent database 3.9.1 (Allocation, cut-off by classification) (Wernet et al., 2016) unless otherwise specified. Table A.4 displays the main inventory data for the ABC-Salt process.

2.6.1. Goal and scope definition, functional unit, life cycle impact assessment

The goal of this LCA is an environmental impact analysis of the ABC-Salt SAF and comparison to traditional fossil kerosene. 1 MJ_{LHV} of fuel is chosen as the functional unit and the LCA is performed from well-to-wheel following the attributional approach. The geographical scope is Sweden, however, most life cycle inventory (LCI) are on a European basis. The life cycle impact assessment (LCIA) is performed with the Environmental Footprint method *EF v3.0 no LT* (Fazio et al., 2018) because it is one of the newest methods and was developed by the European Commission for the European context.

2.6.2. ABC-salt plant, transportation and wastewater treatment

The equipment components for the ABC-Salt plant, except for the ones related to hydrogen, are not included in the LCI because their construction materials and amounts could not be estimated reliably. Since the ABC-Salt process is integrated with a pulp mill process, the plant is located in Sweden right next to the pulp mill. Therefore, transport distance between pulp mill and ABC-Salt plant are neglected due to close proximity. For the supply of raw materials respective market activities were selected since they already include generic transport efforts. Wastewater treatment of the aqueous phases separated after the HP and HDO-1/-2 is estimated with a generic wastewater treatment plant operation.

2.6.3. Molten salt and catalyst

Amounts of zinc and hydrochloric acid needed for the production of zinc chloride as part of the molten salt are calculated based on the following chemical equation (Patnaik, 2003):

$$Zn + 2\ HCl \rightarrow ZnCl_2 + H_2 \tag{2.10}$$

The Ni/Mo catalyst for the two HDO units is assumed to consist of 13 $\%_{wt.}$ MoO_3 and 4.03 $\%_{wt.}$ NiO on an Al_2O_3 support (Zhou and Lawal, 2015). Nickel oxide is produced by heating pure nickel powder with oxygen at a temperature above 400 °C (Patnaik, 2003). Only the oxygen uptake from the biosphere is considered for the production while the energy for heating was neglected because of a lack of more detailed information. Spent catalysts is assumed to be sent to a hazardous waste landfill (European Commission, 2014). The total amount needed for the upgrading of the HP oil was estimated in the ABC-Salt project with 4500 $l_{HP\ oil}/kg_{cat}$ and a HP oil density of 1.1 kg/l.

2.6.4. Hydrogen production and recovery

As mentioned in Chapter 2.2 pure hydrogen is provided by an AEL. The electrolyte is a 25 $\%_{wt.}$ KOH solution (Koj et al., 2017) that requires 10 kg deionised water and 0.275 g potassium hydroxide per kg hydrogen produced (Kuckshinrichs et al., 2017). The AEL cell stack construction is based on a 6 MW AEL with four cell stacks and a stack life time of 10 years (Koj et al., 2017). The hydrogen recovery membrane is assumed to be a polysulfone hollow fiber membrane (Baker, 2012) for the LCA instead of a polyimide membrane as in the economic calculation due to data availability. Membrane production is estimated and scaled from laboratory-scale fabrication (Yadav et al., 2021) and the membrane's lifetime is set to 5 years (Scholes et al., 2015).

2.6.5. Fuel distribution and combustion

ABC-Salt fuel is assumed to be already at jet fuel grade and can hence be directly distributed analogue to fossil kerosene distribution. The combustion of ABC-Salt SAF is approximated with kerosene combustion in a medium haul passenger aircraft. Due to lack of actual combustion data for the ABC-Salt fuel, emissions are based on fossil kerosene combustion emissions but with biogenic carbon dioxide and monoxide instead of the fossil ones. For the comparison with fossil fuel, combustion of fossil kerosene is assumed to take place in the same medium haul passenger aircraft. The aircraft itself is herby neglected.

2.6.6. Pulp mill multi-functionality and allocation

Since the pulp mill process with lignin extraction is a multi-output process, allocation needs to be performed to obtain a single-output process with only lignin as its product. Two different allocation methods are considered in this publication: marginal allocation and classic energetic/economic allocation. Further lignin allocation methods and their effect on LCIA results can be found in Hermansson et al. (2020).

Marginal allocation allocates the difference in environmental impacts from before and after introducing lignin extraction at a Kraft pulp mill to lignin. The classic energetic/economic allocation considers the lignin extraction at the pulp mill on a system level. Thus, the pulp mill with lignin extraction is investigated as a whole and environmental impacts are allocated to all products (pulp, power, tall oil, turpentine and lignin) according to their energetic or economic value with respect to the total product output. The choice of allocation method depends on whether the lignin extraction is viewed as an additional process step separate from the actual pulp process (marginal approach) or as an integral part of the pulp mill process (energetic/economic allocation). For the latter energetic and economic allocation are considered as a pulp mill strives to both maximise its energetic efficiency as well as minimize its cost and the resulting allocation factors differ by a factor of two, significantly impacting the results. The allocation factors for lignin as well as the input parameters for their calculation can be found in SI-Table 5.10 and 5.11.

2.6.7. Lignin

The life cycle inventories of lignin for both allocation methods are displayed in SI-Table 5.8 and 5.9. The input values for both inventories stem from the pulp mill model described in Chapter 2.3 with additional transport of 350 km for chemicals/wastes and 100 km for pulpwood. For marginal allocation two different electricity sources, namely Swedish hydro (run-of-river) and grid mix electricity, are investigated as substitution for the reduction in electricity output of the pulp mill. While lime demand and ash production decrease with Kraft lignin extraction, sodium hydroxide consumption and green liquor dregs production increase and additional chemicals like carbon dioxide and sulfuric acid are required for lignin extraction. The CO_2 uptake by the pulpwood is not allocated according to any of the aforementioned methods but is rather assumed to be offset by biogenic CO_2 emissions during the production and use phase (CO_2 uptake: $-1\ kg_{CO_2\text{-eq.}}/kg_{CO_2}$; CO_2 emission: $+1\ kg_{CO_2\text{-eq.}}/kg_{CO_2}$).

2.7. Combined TEA and LCA

The main objective of alternative fuels, namely the reduction of global warming potential compared to fossil fuels, can be contrasted with the increase in net production costs in the greenhouse gas abatement costs (*GHG abatement cost*):

$$GHG\ abatement\ cost = \frac{NPC_{ABC-Salt\ Fuel} - NPC_{Fossil\ Fuel}}{GWP_{Fossil\ Fuel} - GWP_{ABC-Salt\ Fuel}} \tag{2.11}$$

where $NPC_{ABC-Salt\ Fuel}$ and $NPC_{Fossil\ Fuel}$ are the net production cost and $GWP_{ABC-Salt\ Fuel}$ and $GWP_{Fossil\ Fuel}$ the global warming potentials of the respective fuels. For $NPC_{Fossil\ Fuel}$, the average jet fuel price in 2020 of 0.29 $€_{2020}/l$ (U.S. Energy Information Administration EIA, 2020) is assumed and $GWP_{Fossil\ Fuel}$ is estimated with 94 $g_{CO2\text{-eq.}}/MJ$ from the RED II (European Parliament, 2018). The lower heating values of the fossil fuel and ABC-Salt fuel are 35.3 MJ/l (Engineering ToolBox, 2003) and 33.71 MJ/l (42 MJ/kg and 802.55 kg/m^3), respectively.

3. Results and discussion

Within this chapter the technical, economic and ecological key performance indicators are discussed for the sustainable aviation fuel (SAF) produced through the ABC-Salt process. The resulting ABC-Salt fuel is already in quite good agreement with current jet fuel specifications with a few exceptions like flash point, final boiling point and freezing point. The full product property comparison was reported in Adelung et al. (2022).

3.1. Technical evaluation

Since the ABC-Salt process is integrated with a pulp mill, exchanges with the pulp mill constitute an important factor for the mass and energy balance of the process. Roughly 700 kg/h of gases with a lower heating value (LHV) of 42.6 MJ/kg are separated from the ABC-Salt process and transferred to the pulp mill. The main component is methane (35 $\%_{wt.}$) followed by C_8H_{16} (13 $\%_{wt.}$), C_7H_{14} (11 $\%_{wt.}$), C_6H_{12} (10 $\%_{wt.}$), H_2O (9 $\%_{wt.}$), CO_2 (8 $\%_{wt.}$), H_2 (6 $\%_{wt.}$), C_8H_{10} (5 $\%_{wt.}$) and 3 $\%_{wt.}$ of remaining components. Additionally, 9 kg/h of char (LHV: 30.5 MJ/kg) are generated and also transferred to the pulp mill. Pinch analysis (SI-Fig. 6.1) indicates that the ABC-Salt process is an exothermic process. As a result, 5.9 t/h of steam (@ 10 bar and 180 °C) can be produced from the heat of the ABC-Salt plant, which can contribute to the electricity generation at the pulp mill.

The hydrogen, carbon and overall mass balances are shown in Table 5. The balances include the hydrogen from the electrolyser instead of the deionised water (10.11 $kg_{deionised\ water}/kg_{H2}$) since the excess water exits the model boundaries unchanged. Almost half of the hydrogen (48 %) that enters the ABC-Salt process is incorporated in the fuel product, while 28 % are transferred to the pulp mill for combustion and the remaining 24 % end up in the aqueous phase, mostly in the form of water from, e.g., the hydrodeoxygenation reactions. Roughly 8.6 kg_{H2} are required to process 1 kg of dry lignin. Already 3.4 $kg_{H2}/kg_{lignin,dry}$ are necessary stoichiometry wise in order to remove the oxygen contained in the lignin feed, which is essential if the product is to be used as jet fuel. Moreover, hydrogen is required for the cracking and saturation reactions. Nevertheless, hydrogen is also lost to the pulp mill as gas, in pure form or compound, and to a minor extent in the char.

Carbon enters the system boundaries in the form of dry lignin. A large amount of this carbon also ends up in the fuel product (78 %), whereas losses occur mainly through the gases that are sent to the pulp mill. In comparison, catalytic fast pyrolysis with subsequent hydrotreatment and the IH2 process can only reach carbon efficiencies of up to 50 % due to significant quantities of coke being formed on the surface of the catalyst (Venderbosch, 2015). The ABC-Salt process on the other hand only shows very low char yields (less than 3 g char on 1 kg of dry lignin feed). Two studies, which utilise catalytic hydrotreatment to produce kerosene-like fuel, mention carbon efficiencies closer to the one observed for ABC-Salt, namely 78 % (Piskorz et al., 2002) and 81 % (Stone et al., 2022). However, both refer to a more depolymerized lignin derived oil instead of technical lignin as feedstock.

From an overall mass balance perspective, the biomass to hydrocarbon yield is slightly lower than the ones in the formerly mentioned two studies with 60 $\%_{wt.,dry\ lignin}$ compared to 60–65 $\%_{wt.,dry\ feed}$ (Piskorz et al., 2002) and 61 $\%_{wt}$ (Stone et al., 2022) but it should be taken into consideration that the lignin raw material differs. In comparison to other existing comparable technologies the hydrocarbon yield is about twice as high. IH2, for instance, has a hydrocarbon yield of 25–28 $\%_{wt.}$ using wood as input (Marker et al., 2011).

The process requires a total electrical energy input of 18.8 MW_{el}, ~81 % for electrolysis and ~19 % for compression. The dry lignin feed has an LHV of 27.8 $MJ/kg_{lignin,dry}$ in the Aspen Plus® simulation, which is higher than the analytical LHV due to the approximation of lignin as $C_{20}H_{24}O_6$. The simulated process produces almost 2 t/h of fuel with an LHV of 42 MJ/kg_{Fuel} and a density of 802.55 kg/l_{Fuel}. With Equation (2.7) this results in an energy efficiency of 52.5 $\%_{LHV}$, which is similar to that of other certified SAF routes (~50 $\%_{LHV}$ from biomass to fuel) (de Jong et al., 2015). Moreover, the energy efficiency is also in the range of other catalytic hydropyrolysis processes for hydrocarbon production from lignocellulosic biomass (13–63 $\%_{HHV}$) (Kan et al., 2020) and slightly higher than the one from power-to-liquid SAF processes (22.6–52.2 $\%_{LHV}$) (Rojas-Michaga et al., 2023).

3.2. Economic evaluation

A comprehensive economic assessment of the net production cost was conducted for both lignin and the ABC-Salt SAF, the results of which are presented and discussed hereinafter.

3.2.1. Lignin

The extraction of lignin leads to additional cost for the pulp mill compared to a pulp only operation. The most obvious costs for lignin production are the investment cost of the LignoBoost plant and the chemicals (CO_2 and H_2SO_4). However, there are two additional pulp mill consequential costs that require a more detailed explanation.

Table 5
Mass balances of the ABC-Salt plant.

Hydrogen Balance					
In	kg/h	%	Out	kg/h	%
Lignin, dry	218	41.2	Fuel	254	48.1
Lignin, moisture	32	6.0	Aqueous phase incl. salt	126	23.8
Hydrogen from water electrolysis	281	52.9	Gas to pulp mill	148	28.2
Salt	0	0.0	Char	1	0.1
Carbon Balance					
In	kg/h	%	Out	kg/h	%
Lignin, dry	2166	100.0	Fuel	1693	78.2
Lignin, moisture	0	0.0	Aqueous phase incl. salt	16	0.7
Hydrogen from water electrolysis	0	0.0	Gas to pulp mill	450	20.8
Salt	0	0.0	Char	7	0.3
Mass Balance					
In	kg/h	%	Out	kg/h	%
Lignin, dry	3250	83.3	Fuel	1974	50.6
Lignin, moisture	283	7.2	Aqueous phase incl. salt	1222	31.3
Hydrogen from water electrolysis	280	7.2	Gas to pulp mill	695	17.8
Salt	88	2.3	Char	9	0.2

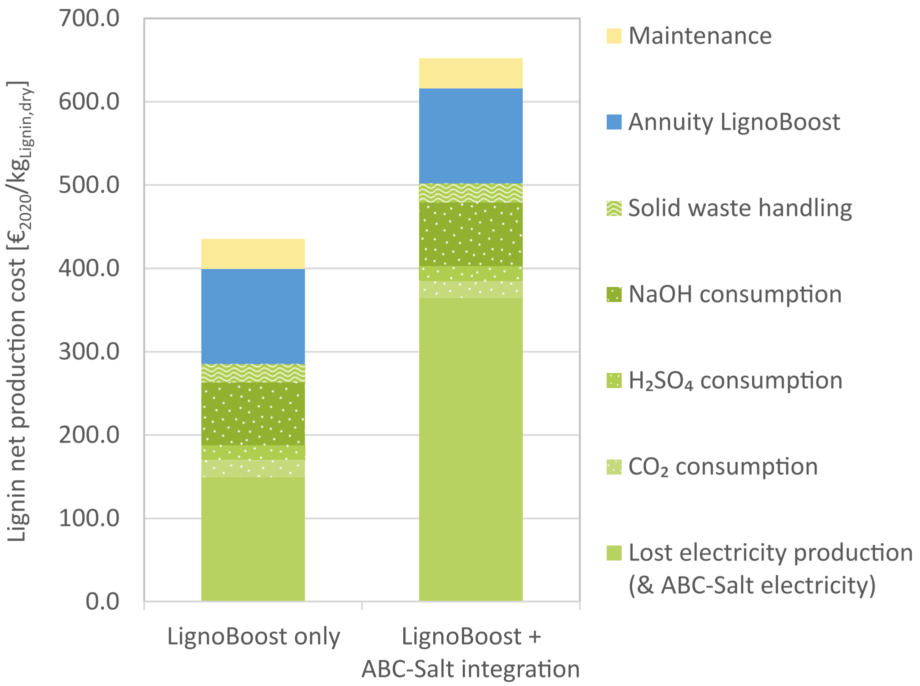

Fig. 3. Pulp mill lignin production cost with the LignoBoost concept without any integration (left) and when integrated with the ABC-Salt process (right).

- Lost power production: In a pulp mill, all black liquor is typically incinerated in the recovery boiler for steam and power production. This results in an energy surplus for the mill and the excess power is sold. However, when part of the lignin is separated less steam and power is produced (6.5 % loss in power production or 11 % based on power sold). The loss of income from sold power is regarded an operational cost in the lignin production.
- NaOH and solid waste handling: The ratio of the two main chemicals in the Kraft pulp process, NaOH and Na_2S, should be kept as stable as possible to not compromise pulp yield and quality. When the acidic and sulphur rich filtrate of the LignoBoost process is returned to the pulp mill, the Na/S balance at the pulp mill is affected. A majority of softwood Kraft pulp mills in Northern Europe already have an excess of sulphur during normal operations. To counteract this imbalance, the purging of the sulphur rich dust from the recovery boiler is increased. However, for every kg of sulphur lost with the dust, there is roughly 2 kg of sodium lost, too. Hence, the makeup of NaOH increases as well. Furthermore, there is additional landfill cost for handling the increased amount of purged recovery boiler dust.

Fig. 3 displays the lignin net production cost (NPC_{Lignin}) for the pulp mill and its composition of sub-costs with and without ABC-Salt process integration. The three most prominent cost factors for NPC_{Lignin} are in descending order the changed revenue from selling of power to the grid, the LignoBoost process investment cost, and the NaOH makeup. The integration of the ABC-Salt process increases NPC_{Lignin} by 33 % from 436 to 652 $€_{2020}/t_{lignin,dry}$ (401 to 600 $€_{2020}/t_{lignin,8\%\ moisture}$). The integration of the ABC -Salt process only has an impact on the pulp mill's energy balance. No further investments are deemed necessary nor will it have any additional effects on the pulp mill's chemical balances. It is obvious that the assumed selling price of power plays a significant role in NPC_{Lignin}. For instance, a 30 % decrease in power price, to 35 €/MWh, would result in NPC_{Lignin} of 549 instead of 652 $€/t_{lignin,dry}$. Furthermore, it should be highlighted that the effects of lignin separation on the mill and the associated production price are going to be unique and need to be evaluated for each specific case since every pulp mill has its own process conditions and black liquor characteristics. Nevertheless, the NPC_{Lignin} values are in good agreement with literature (low purity lignin 50-280 $€/t_{lignin}$, high purity lignin up to 750 $€/t_{lignin}$ and Kraft lignin 250-500 $€/t_{lignin}$) (Ľudmila et al., 2015; Gosselink, 2011).

3.2.2. *Sustainable aviation fuel*

More than half of the total production costs (TPC) for the ABC-Salt fuel shown in Fig. 4 stem from the raw materials and utilities (55 %). The main cost contributor to the raw materials and utilities is the lignin. Stack replacement, salt and deionised water only constitute a minor share and the remaining cost for HCl, membrane replacement, cooling water and KOH are almost negligible. The second largest contributor to the TPC is the annuity (21 %), which is closely related to the fixed capital investment (FCI). The main cost contributors to the FCI are HDO-1, membrane, electrolyser and pyrolysis. HDO-2 is less costly than HDO-1 as the throughput in HDO-1 is substantially larger (37 t/h vs. 3 t/h), mainly because of the liquid recycle stream. In total, the fuel net production cost (NPC_{Fuel}) amount to 1.66 $€_{2020}/l_{Fuel}$ (2.07 $€_{2020}/kg_{Fuel}$, 177.0 $€_{2020}/MWh_{Fuel}$). A break-down of NPC_{Fuel} can be found in SI-Fig. 7.1. If the stabilised HP oil in the liquid recycle stream could act as a liquefaction agent in addition to simple phenols and, hence, less liquid needs to be recycled in total, NPC_{Fuel} would already drop to 1.54 $€_{2020}/l_{Fuel}$.

Another scenario is the reforming of the ABC-Salt's gases, mainly its methane (245 kg/h), instead of sending it to the pulp mill for electricity generation. To estimate the cost reduction potential, a simplified calculation was performed. The conversion rate from methane (50 MJ/kg (Engineering ToolBox, 2003)) to hydrogen (120 MJ/kg (Engineering ToolBox, 2003)) was assumed to be around 75 % based on lower heating value (Antonini et al., 2020), with the remaining 25 % providing the heat for the steam methane reforming. The reformer cost was estimated based on the heat duty of 850 kW (Table A.1) and the alkaline electrolyser size was simultaneously reduced by 4.1 MW to a total of 10.9 MW. When considering the reduction in electricity consumption by the electrolyser (−0.11 $€_{2020}/kg_{Fuel}$) and the loss of electricity production form the gas (0.08 $€_{2020}/kg_{Fuel}$), NPC_{Fuel} overall reduces by 0.03 $€_{2020}/l_{Fuel}$ to 1.63 $€_{2020}/l_{Fuel}$. However, one needs to keep in mind that the required reformer is actually quite small and, hence, out of range for the applied cost function. Moreover, in reality all hydrocarbons in the gas stream would probably be reformed, not just the

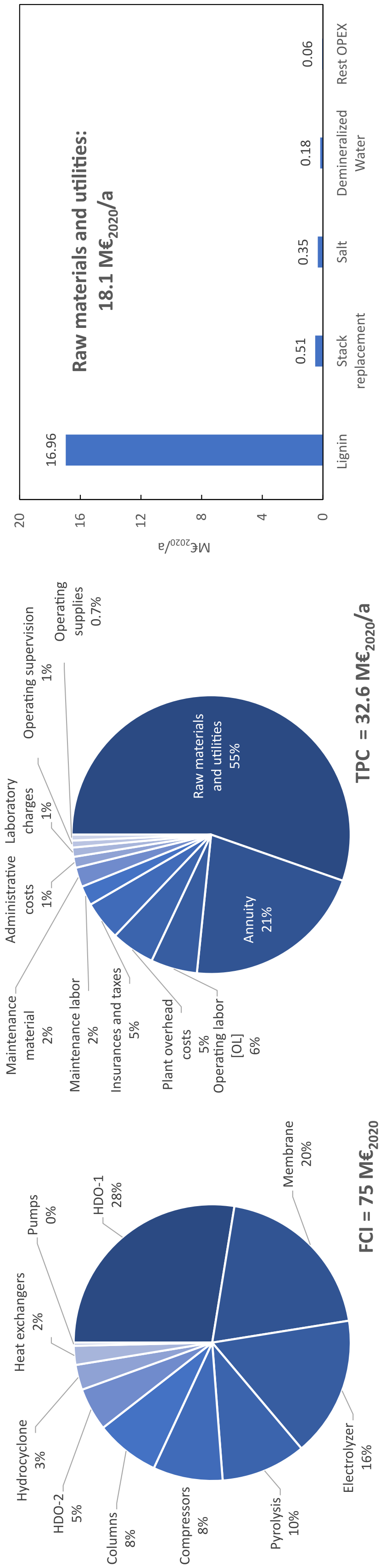

Fig. 4. Economic cost break-down for fixed capital investment (FCI), total production costs (TPC), and raw materials and utilities of the ABC-Salt process for a yearly product output of 15.8 kt/a.

methane, which is more complex to calculate since it requires an additional pre-reformer and the overall heating demand is harder to estimate.

Even though NPC_{Fuel} is higher than the fossil jet fuel price of 0.29 $€_{2020}$/l (U.S. Energy Information Administration EIA, 2020), it is still below average power-to-liquid SAF prices of ~2 $€_{2019}$/l for direct air capture and Fischer-Tropsch synthesis at a similar electricity price as for NPC_{Fuel} (Seymour et al., 2024). Furthermore, NPC_{Fuel} is within the minimum fuel selling price (MFSP) range for American Society for Testing and Materials (ASTM) certified SAF production routes ($ 1.12–3.99/l) (Watson et al., 2024). In comparison to an assessment by Jafri et al. (2020) for biofuel produced from pulp mill lignin or black liquor, NPC_{Fuel} is higher because of mainly two underlying assumptions. The pulp mill configuration closest to this publication is the model mill, which yielded the following MFSPs for the two closest biofuel process configurations: ~132 $€_{2017}/MWh_{biofuel}$ for lignin liquefaction and hydrotreatment with hydrogen from electrolysis (configuration 1b in Jafri et al.), ~95 $€_{2017}/MWh_{biofuel}$ for black liquor gasification and methanol to fuel synthesis with hydrogen from electrolysis (configuration 2b in Jafri et al.). The two major contributors to the difference in production cost are the lower electricity price of 33.5 €/MWh in Jafri et al. compared to 48.8 €/MWh in this publication and including only one cost factor for indirect OPEX, namely 4 % for operation and maintenance. When the production costs of this publication are adjusted to these values, NPC_{Fuel} would be similar to process configuration 1b with around 136 $€_{2020}/MWh_{Fuel}$. The same were true in comparison to configuration 2b if no lignin needed to be extracted and black liquor could be directly used in the ABC-Salt process reducing the production cost to roughly 95 $€_{2020}/MWh_{Fuel}$ by additionally excluding the cost for lignin extraction (41 $€_{2020}/MWh_{Fuel}$).

3.3. Ecological evaluation

The life cycle assessment comprises an in-depth global warming potential contribution analysis and comparison with fossil jet fuel for 16 impact categories.

3.3.1. Global warming potential

The global warming potential (GWP) of the ABC-Salt fuel depicted in Fig. 5 strongly depends on the GWP allocated towards lignin and hence also on the chosen allocation method. Around 74–90 % of the fuel GWP is ascribed to lignin (green coloured parts) with economic allocation having the lowest and marginal allocation with grid mix electricity having the highest lignin contribution. The GWP of zinc chloride production and kerosene distribution is the same for all 4 bars since only the lignin GWP is influenced by the changes in allocation method.

For marginal allocation the substituted electricity as well as the chemical production of liquid carbon dioxide and sodium hydroxide have a major impact contribution. When the loss in electricity generation at the pulp mill is substituted by renewable electricity like hydro power with one of the lowest GWPs instead of Swedish grid mix electricity, the GWP of the fuel is reduced by 30 %. A minor GWP contribution is also provided by the transport for the additional chemicals needed for the Kraft lignin extraction.

When energetic or economic allocation is applied instead, the GWP is overall lower than with marginal allocation and the impact contributions are more diverse. Around 25 % of the lignin GWP are associated with pulp wood harvesting (monochrome dark green), 46 % with production of chemicals for the pulp mill and Kraft lignin extraction process (dotted greens), 14 % with transport of pulp wood and chemicals (striped greens), 8 % with waste treatment (waved greens) and the remaining 7 % with some smaller contributions from further chemical productions and waste treatments (monochrome light green). The lignin GWP contribution for energetic allocation is overall higher than for economic allocation because the allocation factor is 1.7 times larger (5.6 % for energetic allocation vs. 3.2 % for economic allocation).

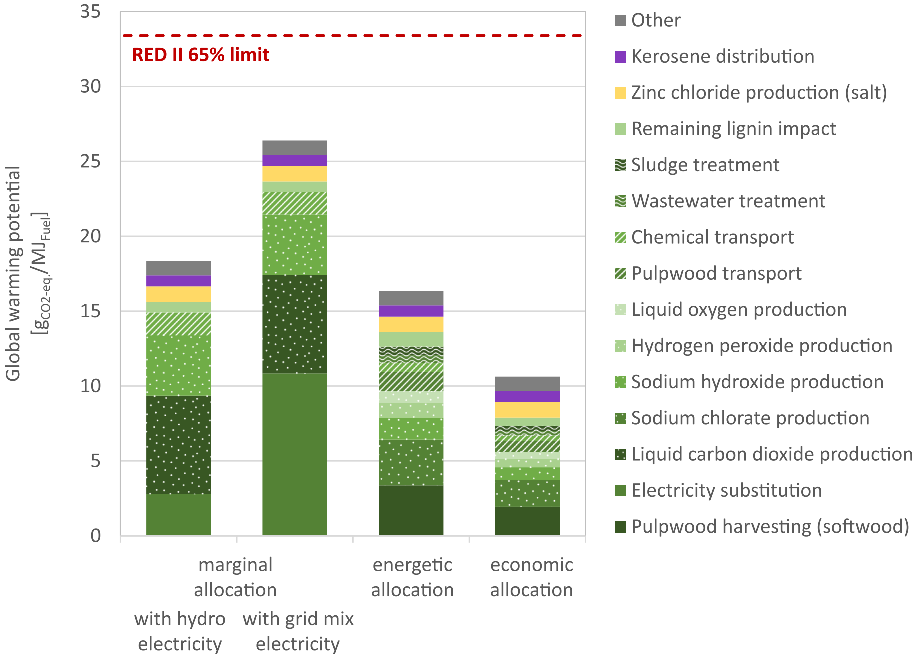

Fig. 5. Global warming potential break-down with four different lignin allocation approaches. Green colours belong to Kraft lignin production at pulp mill.

Overall, the ABC-Salt fuel indicates an impact reduction compared to fossil fuel of at least 72 % for marginal allocation with grid mix electricity up to 89 % for economic allocation of the lignin. Therefore, the 65 % limit set by the RED II can be reached. A break-down of impact contribution for the remaining 15 impact categories of the Environment Footprint method can be found in SI-Fig. 8.1. Whether fuel production is the best application for lignin in terms of GWP savings compared to other lignin derived products (Moretti et al., 2021) could be determined by a resource-perspective LCA (Hanssen and Huijbregts, 2019), which is beyond the scope of this publication.

3.3.2. *Fossil jet fuel comparison*

Compared to fossil kerosene the ABC-Salt fuel exhibits an impact reduction in about 3 categories including the GWP, similar environmental impact in 3, a slight increase in another 4 and a big increase in the remaining 6 impact categories. Fig. 6 illustrates these findings for the ABC-Salt fuel as a share of the environmental impacts for fossil kerosene where a value smaller one signifies an impact reduction and above one an impact increase. In the following paragraphs a few key points will be highlighted.

Whether a reduction or increase can be observed not only depends on the whole fuel production chain but also, at least for some categories, on the chosen allocation method for lignin production at the pulp mill. When less environmental impacts are allocated to lignin and in consequence to the fuel, more will be allocated to the remaining products at the pulp mill (electricity, pulp, tall oil and turpentine), keeping the environmental impacts of the overall system constant. Categories affected by the chosen lignin allocation method include fossil resource

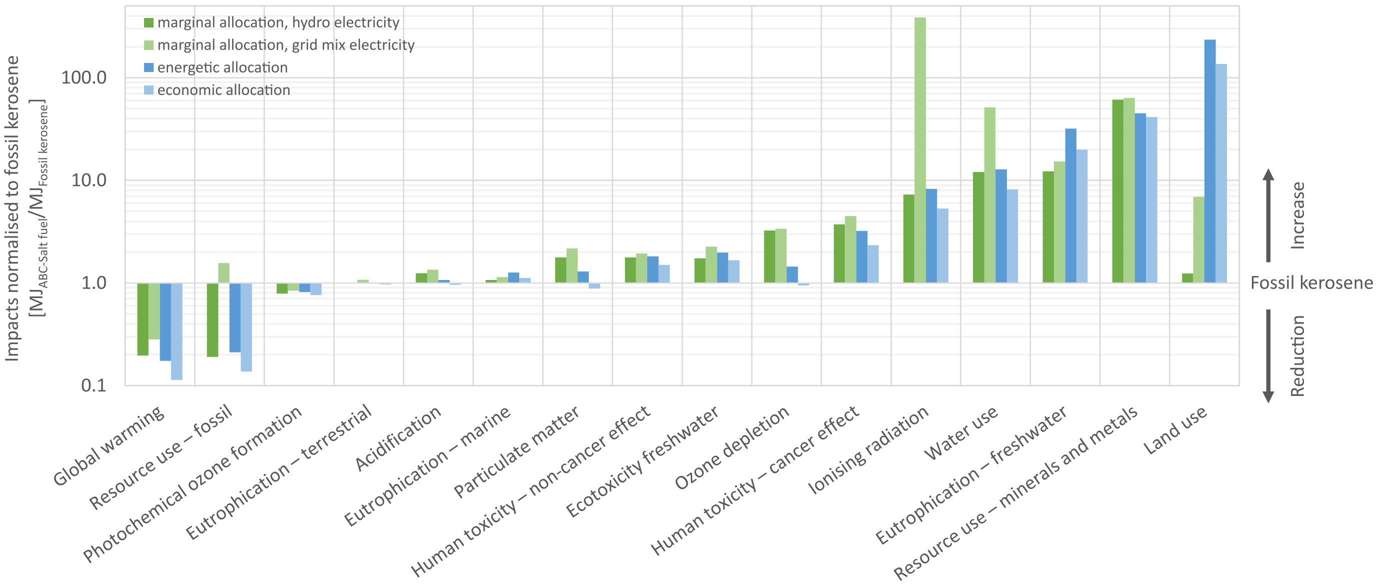

Fig. 6. Environmental impact comparison of ABC-Salt fuel and fossil kerosene with four different lignin allocation approaches.

use, acidification, particulate matter, and ozone depletion. For the first category the substitution with Swedish grid mix electricity in marginal allocation is the reason for the impact increase instead of reduction. More specifically, the nuclear electricity portion of the grid mix causes a high impact in this category through uranium usage. For the latter three categories, only economic allocation exhibits an impact reduction as less environmental impact, especially from sulfuric acid and sodium hydroxide production, are allocated towards lignin. Sulfuric acid production with its sulphur oxide emissions has a particular strong impact on acidification and particulate matter, while sodium hydroxide production contributes highly to ozone depletion with its tetrachloromethane emissions.

There are three more categories with a high contrast between the allocation methods for lignin: ionising radiation, water use, and land use. The nuclear electricity generation in marginal allocation with grid mix electricity is both responsible for the peak in ionising radiation and contributing to the elevated impact in water use. Besides nuclear electricity, the mayor contribution to water use stems from hydro reservoir electricity. This hydro electricity type is associated with a higher water use than the more common hydro run-of-river electricity in Sweden, which is used in the marginal allocation method with hydro electricity. Land use impact increase for energetic/economic allocation is almost entirely associated with the land use from pulpwood, which is excluded in the marginal approach as the pulp wood intake to the pulp mill does not increase by the Kraft lignin extraction. The reason why the marginal allocation with grid mix electricity still shows a more significant impact increase in contrast to the one with hydro power is related to the production of electricity from wood chips in the Swedish grid.

Some of the impact increases compared to fossil kerosene are to be expected with regards to biofuels when impacts from the biomass growth phase are ascribed to the fuel, namely the ones in the categories water use and land use (Weyand et al., 2023). Interestingly, the impact increase also occurs for marginal allocation were no impact from the biomass itself is allocated to the lignin and hence to the fuel but is rather a product of the electricity substitution. An impact increase in the minerals and metals resource use category is to be expected as well, simply because the process chain for biofuel production requires more processing steps than for fossil fuels. Furthermore, higher or similar impacts compared to fossil kerosene are either not avoidable or overestimated in categories with a significant contribution from kerosene combustion because combustion emissions of the ABC-Salt fuel are based on the fossil kerosene ones. These emissions in addition to the longer production chain of sustainable aviation fuel inevitably results in higher impacts. Here, it effects the categories photochemical ozone formation, terrestrial eutrophication, acidification, marine eutrophication, particulate matter and both human toxicity categories.

3.4. Sensitivity analysis with combined TEA and LCA

Since hydrogen and its recovery rate is an important design parameter which indirectly influences the lignin cost and environmental impact through changes in electricity demand, a sensitivity analysis was conducted. The effect of the hydrogen recovery rate on the GWP, NPC and GHG abatement cost is shown in Fig. 7. Additionally, the influence of the hydrogen source on these three key figures was investigated by replacing the green hydrogen from electrolysis with grey hydrogen bought from the grid (1.41 €/kg_{H2} (Hydrogen Europe, 2021), ecoinvent dataset ‘hydrogen production, steam reforming’ (Wernet et al., 2016)). The star marks the results for a hydrogen recovery rate of 98 % that was used as the base value for the previous chapters. Only the energetic allocation case for lignin is discussed in this chapter while the other allocation cases are addressed in SI-Chapter 9.

When the hydrogen recovery rate is decreased towards 70 %, the NPC slightly increases. More fresh hydrogen needs to be produced with the electrolyser which directly correlates with the electricity supply by the pulp mill and in turn raises the cost for lignin. However, very high recovery rates are also not favourable for the NPC because the membrane area grows into infinity and with it the cost. The same behaviour can be observed for grey hydrogen although with overall slightly lower NPC for the fuel as grey hydrogen comes with lower cost.

The reverse is true for overall fuel GWP as grey hydrogen is associated with a much higher GWP than green hydrogen production. The positive effect of higher hydrogen recovery rates on the GWP, however, is only discernible for grey hydrogen even though the same applies for green hydrogen. The decreased fresh hydrogen demand lowers the electricity supply by the pulp mill for green hydrogen production and reduces the GWP contributed by grey hydrogen from steam methane reforming. Overall, 70 % hydrogen recovery can still achieve the required RED II GWP savings with green hydrogen while an ABC-Salt fuel produced with grey hydrogen does not fulfil this requirement even with high hydrogen recovery rates. Even worse, a 70 % hydrogen recovery rate results in a GWP that is higher than the fossil fuel one. The membrane area going to infinity for very high hydrogen recovery rates effects the GWP only slightly.

For the combination of the two key figures in the GHG abatement cost the effect of hydrogen recovery is quite limited for green hydrogen

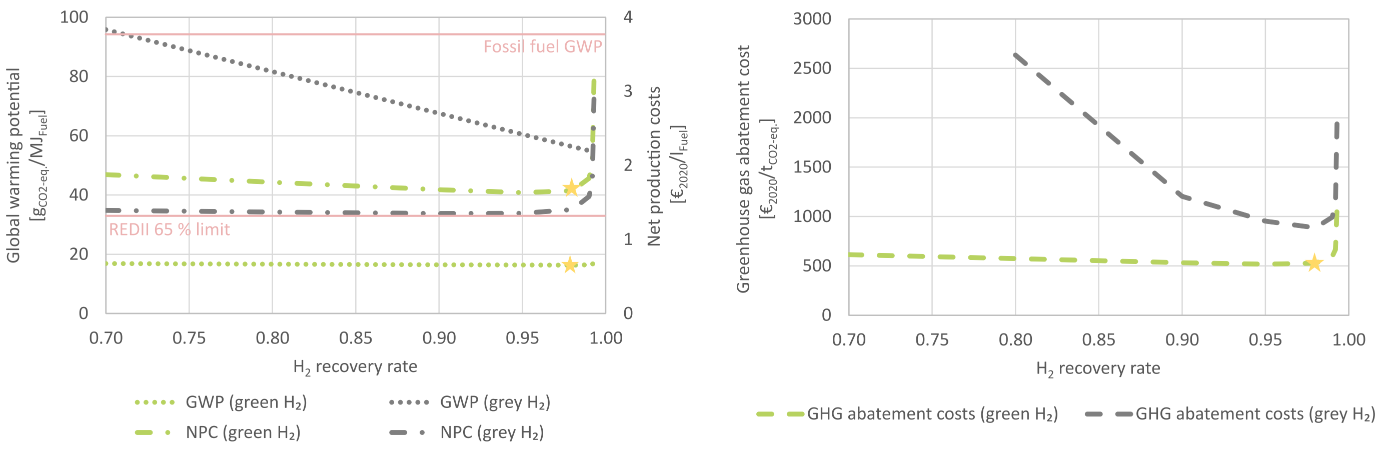

Fig. 7. Sensitivity analysis of hydrogen recovery rate and hydrogen source for GWP, NPC and GHG abatement cost (energetic allocation of lignin production). Star indicates the base case conditions.

but significant for grey hydrogen with the exception of very high recovery rates. This results in an optimal hydrogen recovery rate between 95 and 98 % for both NPC and GWP in this process setup. Although green hydrogen production is associated with higher cost, its use is altogether favourable in terms of GHG abatement cost due to its lower GWP. To ensure a cost competitive market entry, a minimum emission trading system (ETS) CO_2 price of 500 €/$t_{CO2\text{-eq.}}$ would be currently necessary. In the future, technological improvements, reductions in raw material costs and regulatory requirements are also conceivable to improve the ABC-Salt fuel's competitiveness.

4. Summary

This work investigated a novel concept (ABC-Salt process) to produce sustainable aviation fuels (SAF) from lignin via molten salt catalytic hydropyrolysis and catalytic hydrodeoxygenation with respect to material and energy efficiency as well as from an economic and ecological perspective. Therefore, a comprehensive techno-economic assessment (TEA) and life cycle assessment (LCA) was conducted. The process generates hydrocarbons with a middle distillate fraction already in fairly good agreement with current jet fuel specifications. By integration into the lignin providing pulp mill process, the ABC-Salt process benefits from green electricity supply. In turn, the by-products gas, char and heat/steam are sent to the pulp mill for electricity generation. Two notable novelties of the ABC-Salt process are the use of molten salt as a catalyst and the recycling of partial amounts of the first hydrodeoxygenation (HDO-1) product as liquefaction agent for hydropyrolysis. Firstly, this allows for low char yields, which leads to a high carbon efficiency of 78 %, and secondly it improves the feeding of the lignin to the pressurized units and ensures good heat transfer to the otherwise solid feed stream. The energy efficiency of the ABC-Salt (52.5 $\%_{LHV}$) is furthermore on the higher end of other SAF production routes.

Net production cost of the fuel are at 1.66 $€_{2020}/l_{Fuel}$ with a lignin price of 612 $€_{2020}/t_{lignin,dry}$ incl. electricity delivered to the ABC-Salt process (48.8 €/MWh_e). The main cost contributor is the lignin cost itself which is highly dependent on the loss of income from power generated at the pulp mill. A quick sensitivity analysis shows that lignin cost below 5 €/t would be necessary in order for the fuel cost to drop below 1 €/kg or 0.8 €/l if the equipment cost remain the same. Because of the multifunctionality of the pulp mill process, allocation was applied to the Kraft lignin production at a pulp mill within the LCA. The choice of allocation method strongly affects the resulting global warming potential (GWP) as well as multiple other environmental impacts. Consequently, the GWP savings in relation to fossil fuel range between 72 and 89 %, which is still well above the RED II biofuels threshold. Higher impacts with categories like water and land use are to be expected with biofuels but impact increases in other impact categories should be kept in mind and potentially improved during further development. Because of the large quantities of hydrogen required for deoxygenation of the fuel, hydrogen recovery plays an important role in reducing both net production cost and environmental impacts with favourable recovery rates being in the range of 95–98 %. In order to produce cost competitive jet fuel with low greenhouse gas emissions through this novel process concept, a ETS CO_2 price of 500 €/$t_{CO2\text{-eq.}}$ would be currently necessary.

5. Outlook

To further improve the economic viability of the ABC-Salt process, utilising the whole HDO-1 product as liquefaction agent instead of just simple phenols and lowering the liquefaction agent to lignin ratio should be investigated. By broadening the range of HDO-1 products that can be utilised as liquefaction agents or by reducing the required liquefaction agent amount, the liquid recycle stream could be drastically reduced, which in turn decreases the equipment sizes and, hence, equipment cost. Furthermore, from the pulp mill's side installing an internal sulfuric acid plant should be considered to recover the sulphur in its off-gases for H_2SO_4 production (Valmet, 2020). Although H_2SO_4 consumption itself is not a significant lignin cost contributor, removing the sulphur with the off-gases creates a new purging point for sulphur that is much more selective than purging through the recovery boiler ash. This leads to considerable savings in the cost for NaOH makeup as well as solid waste handling of purged recovery boiler ash, which potentially reduces the pulp mills environmental impacts as well. Finally, test runs in a continuous ABC-Salt pilot plant are necessary to validate the TEA and LCA results, which currently rely on a considerable number of assumptions and therefore represent a best-guess.

CRediT authorship contribution statement

Julia Weyand: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Sandra Adelung:** Writing – original draft, Visualization, Validation, Methodology, Formal analysis, Data curation, Conceptualization, Investigation. **Johan Wallinder:** Writing – original draft, Visualization, Methodology, Investigation, Formal analysis. **Balaji Sridharan:** Writing – original draft, Visualization, Investigation, Formal analysis. **Robbie Venderbosch:** Writing – review & editing, Writing – original draft, Funding acquisition. **Hero J. Heeres:** Writing – review & editing, Writing – original draft, Project administration, Funding acquisition. **Ralph-Uwe Dietrich:** Writing – review & editing, Supervision, Resources, Funding acquisition.

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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Appendix B. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2024.144559.

Appendix A

A.1 Economic equations

The annuity (*ACC*) is calculated from the fixed capital investment (*FCI*), the interest rate (*IR*), the plant operating time (*N)* and the working capital share (x_{WC}):

$$ACC = FCI \times IR \times \left(\frac{(1+IR)^N}{(1+IR)^N - 1} + \frac{x_{WC}}{1 - x_{WC}} \right) \tag{A.1}$$

The fixed capital investment (*FCI*) is calculated based on the according capital cost factors ($F_{\text{eco},i,j}$), and the purchased equipment cost (EC_i):

$$FCI = \sum_{i=1}^{m} EC_i \times \left(1 + \sum_{j=1}^{10} F_{\text{eco},i,j}\right) \times \left(1 + \sum_{j=11}^{12} F_{\text{eco},i,j}\right) \tag{A.2}$$

For the purchased equipment cost (EC_i), the purchased equipment cost of the reference ($EC_{\text{Ref,i}}$) is first scaled from the reference capacity ($S_{\text{Ref},i}$) to the actual capacity (S_i) derived from simulation with the dimensioning factor (d_i) and then adjusted to the base year 2020 with the chemical engineering plant cost index (*CEPCI*), as described by the following equation:

$$EC_i = EC_{\text{Ref,i}} \times \left(\frac{S_i}{S_{\text{Ref},i}}\right)^{d_i} \times \left(\frac{CEPCI}{CEPCI_{\text{Ref,i}}}\right) \tag{A.3}$$

The *CEPCI* is compiled on a US$ basis and was 596.2 for the base year 2020.

Direct operational expenditures ($OPEX_{direct,i}$) are calculated by multiplying the stream quantities (m_i) with the market price for the raw material, by-product or utility ($C_{R\&B\&U,i}$) adjusted to the base year 2020 with the commodity price index (*CPI*):

$$OPEX_{\text{direct},i} = m_i \times C_{\text{R\&B\&U,i}} \times \left(\frac{CPI}{CPI_{\text{Ref,i}}}\right) \tag{A.4}$$

Indirect operational expenditures ($OPEX_{indirect,i}$) such as administrative costs and maintenance are calculated based on operational cost factors ($F_{\text{ecoII,j}}$) and their respective basis (B_j):

$$OPEX_{\text{indirect},j} = B_j \times F_{\text{ecoII,j}} \tag{A.5}$$

In addition to the net production costs, the total production costs (*TPC*) are defined as:

$$TPC = NPC \times \dot{m}_{\text{fuel/lignin,dry}} \tag{A.6}$$

A.2 Economic input data

Table A.1
Purchased equipment cost assumptions.

Equipment	$EC_{\text{Ref,i}}$	Currency	$S_{\text{Ref,i}}$	Unit_{Ref}	d_i	Year_{Ref}	Exchange rate for Year_{Ref} (€/US$) [7]	$CEPCI_{\text{Ref,i}}$ [8]	*Refs.*
Pumps [1]	Potential function[1]					2002		395.6	Peters et al. (2003)
AEL	1.02	Mio €	1	MW	0.85	2015	0.9013	556.8	Kuckshinrichs et al. (2017)
HP [2]	0.07	Mio US$	0.24	t/h feed	0.2	2002		395.6	Peters et al. (2003)
HDO-1 [3]	0.35	Mio US$	0.9745	t/h feed	0.68	2007		525.4	Woods (2007)
HDO-2 [3]	0.35	Mio US$	1.1465	t/h feed	0.68	2007		525.4	Woods (2007)
Hydrocyclone	0.25	Mio €	41.67	m^3/h feed	0.67	2010	0.7543	550.8	Vito (2010)
HEX [4]	Polynomial function[4]					2002		395.6	Peters et al. (2003)
Flashes [5]	Based on height, diameter and pressure[5]					2002		395.6	Peters et al. (2003)
Compressors	5	Mio €	10	MW_{el}	0.67	2010	0.7543	550.8	Hannula (2016)
Membrane	50	US$	1	m^2	1	2018		603.1	Zarca et al. (2018)
Reformer[6]	Potential function[6]					2002		395.6	Peters et al. (2003)

[1] Liquefaction and other pumps potential function for centrifugal pump (US$): 16808.4 * ($S_i$ in m^3/s)$^{0.3614}$; material factor: 2.4 for stainless steel; pressure factor: 1.0 for ≤50 bar, 2.1 for >50 bar, 2.8 for >100 bar, 3.5 for >200 bar.

[2] Autoclave (hydropyrolysis): The reactor volume is calculated from the liquid residence time in the experiments to 51.7 m^3 to process 31 t/h (experiment: 60 g liquid feed/(h*100 ml)). A maximum autoclave size of 7 m^3 is assumed (Peters et al., 2003).

[3] Multitube Fixed Bed Reactors (HDO-1, HDO-2): The reactor volumes are calculated from the residence times in the experiments: 51 g liquid feed/(h*157 ml) for HDO-1 and 60 g liquid feed/(h*157 ml) for HDO-2. The resulting reactor volumes are 92.4 m^3 (HDO-1) and 6.28 m^3 (HDO-2) to process 30 t/h and 2.4 t/h, respectively.

[4] Shell & tube heat exchangers polynomial function (US$): 3853.3 + 201.3 * ($S_i$ in m^2 surface area); temperature range: $-200 < T < 600$ °C; pressure range: $p < 30$ MPa; material: stainless steel; pressure factors: 1.0 for ≤50 bar, 1.16 for >50 bar, 1.24 for >100 bar, 1.31 for >150 bar.

[5] Vertical columns (stainless steel): Cost calculated based on height, diameter and pressure according to Peters et al. (2023).

[6] Reformer furnace (stainless steel tubes) potential function (US$): 515.1 * ($S_i$ in kW heat duty)$^{0.8251}$; heat duty range: $2000 \text{ kW} \leq \dot{Q} \leq 100000 \text{ kW}$; pressure range: <138 bar.

[7] International Monetary Fund and International Financial Statistics (2023) (exchange rate 2020: 0.8755 €/US$).

[8] Maxwell (2023)

Table A.2
Assumed market prices for raw materials and utilities (CPI is on US$ basis).

Utility/Raw material	$C_{R\&B\&U,i}$	$Unit_{Ref}$	$Year_{Ref}$	Exchange rate for $Year_{Ref}$ (€/US$) [2]	$CPI_{Ref,i}$ [3]	Refs.
Lignin (8 % moisture, calculated, see Chapter 3.2)	600.19	€/t	2020			See 2.5.2
Salt	631.45	€/t	2015	0.9013	64.787 ^{E}	Mehos et al. (2017)
Hydrochloric acid (HCl)	0.215	$/kg	2018		87.011^{E}	Liu et al. (2018)
Membrane replacement	0.5	$\$/m^2/a$	2018		87.011 ^{E}	Zarca et al. (2018)
Stack replacement[1]	4.25	€/MWh	2015	0.9013	81.625 ^{NE}	Kuckshinrichs et al. (2017)
Potassium hydroxide (KOH)	2.5	€/kg	2015	0.9013	64.787 ^{E}	Kuckshinrichs et al. (2017)
Deionised water	0.01	€/kg	2015	0.9013	64.787 ^{E}	Kuckshinrichs et al. (2017)
Cooling water	0.005	$€/m^3$	2020			Bürgerschaft Hamburg (2014)

^{E} World Bank Commodity Price Index (CPI) for Energy (2020: 51.912).

^{NE} World Bank Commodity Price Index (CPI) for Non-energy (2020: 84.107).

[1] Total cost for stack replacement for plant lifetime of 25 years. Stack lifetime of 66 700 h → Stack has to replaced twice in plant lifetime.

[2] International Monetary Fund and International Financial Statistics (2023) (exchange rate 2020: 0.8755 €/US$).

[3] World Bank (2021)

Table A.3
Purchased equipment cost and specific cost for consumables associated with the LignoBoost process.

Equipment/Consumable	$EC_{Ref,i}/C_{R\&B\&U,i}$	Currency	$S_{Ref,i}$	$Unit_{Ref}$	d_i	$Year_{Ref}$	Exchange rate for $Year_{Ref}$ (€/US$) [2]	*$CEPCI_{Ref,i}$* [3]	*Refs.*
LignoBoost plant	32[1]	Mio €	50 000	$t_{lignin,dry}/a$	0.6	2013	0.7529	567.6	Stora Enso, 2013
H_2SO_4 (96%)	100			€/t		2020			RISE LignoCity (2020)
NaOH	550			€/t		2020			RISE LignoCity (2020)
CO_2	100			€/t		2020			RISE LignoCity (2020)
Power	48.8			€/MWh		2020			BMWK (2022)
Solid waste handling	100			€/t		2020			Swedish pulp mill (2017)

[1] The total equipment cost of the reference. The investment includes a lignin extraction plant and dryer, lignin dust burners in the lime kilns, and a packing line.

[2] International Monetary Fund and International Financial Statistics (2023) (exchange rate 2020: 0.8755 €/US$).

[3] Maxwell (2023)

A.3 Ecological input data

Table A.4
Life cycle inventory of fuel production through the ABC-Salt process (base case).

Product name	Amount	Unit	Activity/Compartment	Location
Product				
Liquid product (fuel)	1	MJ		SE
Raw materials/utilities				
Lignin	0.0426	kg	See SI-Table 5.8 & 5.9	SE
$ZnCl_2$ (Salt)	$6.45\cdot10^{-4}$	kg	market for zinc (0.48 kg_{Zn}/kg_{ZnCl2}) & market for hydrochloric acid, without water, in 30% solution state (0.535 kg_{HCl}/kg_{ZnCl2})	GLO RER
NaCl (Salt)	$8.62\cdot10^{-5}$	kg	market for sodium chloride, powder [1]	RER
KCl (Salt)	$3.34\cdot10^{-4}$	kg	market for potassium chloride	RER
HCl	$4.13\cdot10^{-4}$	kg	market for hydrochloric acid, without water, in 30 % solution state	RER
Deionised water	0.2264	kg	water production, deionised	Europe without Switzerland
Hydrogen [2]	0.0032	kg	hydrogen production, AEL electrolysis, 6 MW, w/o electricity	RER
Ni/Mo catalyst [3]	$1.26\cdot10^{-5}$	kg	market for molybdenum trioxide (0.132 kg/kg_{cat}) & market for nickel, class 1 (0.0317 kg/kg_{cat}) & market for aluminium oxide, non-metallurgical (0.8277 kg/kg_{cat}) & market for hazardous waste, for underground deposit (1 kg/kg_{cat}) & oxygen (0.0086 kg/kg_{cat})	GLO GLO IAI Area, EU27 & EFTA RER Natural resource, air
H_2 recovery membrane [4]	$2.05\cdot10^{-5}$	m^2	Polysulfone membrane, hollow fiber, production	RER
Electricity	(0.2254)	kWh	from pulp mill, included in Kraft lignin extraction LCI (SI-Table 5.8 & 5.9)	SE
Wastes				
Wastewater	$2.42\cdot10^{-4}$	m^3	treatment of wastewater, average, capacity 1E9 l/year	Europe without Switzerland
Environment				
Cooling water [5]	0.0011	m3	natural resource - in water	
To Pulp Mill				
Char	$1.09\cdot10^{-4}$	kg	Supplied to pulp for electricity generation, included in Kraft lignin extraction LCI (SI-Table 5.8 & 5.9)	SE

(*continued on next page*)

Table A.4 (*continued*)

Product name	Amount	Unit	Activity/Compartment	Location
Gas	0.0083	kg	Supplied to pulp for electricity generation, included in Kraft lignin extraction LCI (SI-Table 5.8 & 5.9)	SE
Low pressure steam	0.0699	kg	Supplied to pulp for electricity generation, included in Kraft lignin extraction LCI (SI-Table 5.8 & 5.9)	SE
Product distribution & combustion				
Kerosene distribution	0.0238	kg	kerosene distribution [6]	Europe without Switzerland
Kerosene burned, passenger aircraft, medium haul	1	MJ	kerosene burned, passenger aircraft, medium haul [7]	GLO

[1] market transport distances taken from (Moreno Ruiz et al., 2018).

[2] based on Koj et al. (2017), full inventory is displayed in the Supporting Information (SI-Table 5.2 & 5.3).

[3] 13.2 $\%_{wt.}$ MoO_3 and 4.03 $\%_{wt.}$ NiO on Al_2O_3 (Zhou and Lawal, 2015), hazardous waste disposal after lifetime (European Commission, 2014).

[4] based on Yadav et al. (2021), full inventory is displayed in SI-Table 5.4.

[5] mostly for cooling and some for production of low-pressure steam.

[6] SI-Table 5.5.

[7] SI-Table 5.6.

Data availability

Data will be made available on request.

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