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Assessing methods for the production of renewable benzene

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ABSTRACT

Benzene is a widely used chemical feedstock without an alternative in polymer and high energy density liquid fuel production. Produced from fossil carbon, benzene consumption contributes to rising atmospheric CO_2 levels at the end of life. Several low maturity routes to produce fossil carbon- free, renewable benzene are being developed, each with merits and shortfalls. However, analysis is lacking to evaluate how these routes compare and assess which show the most potential in a sustainability context. Here, nine diverse approaches to renewable benzene production are evaluated using a multi-step Multi-Criteria Decision Analysis (MCDA) technique across indicators in three sustainability categories: 'People', 'Profit', and 'Planet' (3Ps). Three example scenarios are presented to elucidate how stakeholder preference may inform weighting choices and hence outcome. In all cases, the use of Fe/Fe_3O_4 nanoparticle catalysts with CO_2/H_2 feed consistently ranked highest with HZSM-5 catalyst converting lignin feed ranked second. Notably, these routes are exemplified by the simplicity of their respective processes. However, due to the emerging nature of all routes, assessment rankings are likely to change with developmental research and subsequent scale-up. It is probable that any deployed technology would combine a variety of attributes rather than utilise any single route assessed here. Hence, positive and negative hotspots are identified. For example, Zn-ZrO_2 nanoparticles on HZSM-5 exhibit exceptional catalyst lifetime, while many locations may lack the infrastructure to produce nanocatalysts, restricting choice of route. Therefore, an open-access model included with this work allows new routes to be added, process data to be updated and priorities altered. This enables practitioners to continue to assess new routes and improvements.
Ultimately, the route decision will depend highly on geographic location, local availability of a given feedstock and compatibility with an effective catalyst.

1. Introduction

Benzene, along with derivatives Toluene and Xylene (BTX), account for 24% of the global chemicals market (Hodásová et al., 2015), Fig. 1.1. Benzene is used as a light component in fuels to improve knocking characteristics and increase octane rating. At present, almost all benzene is produced via crude oil refining, unlocking fossil stored carbon and contributing to global warming. Primary chemicals (including benzene) contributed 258 Mt. CO_2 emissions to the atmosphere in 2018, equivalent to 56 million passenger vehicles. The demand for base petrochemical feedstocks is predicted to grow, with Deloitte et al. (2019) expecting increases of 4.4%, 4.1%, 3% and 7.2% for ethylene, propylene, benzene and paraxylene respectively by 2022. This would put global benzene demand at 51 million tonnes per year. In a more sustainable circular economy, alternative renewable carbon based feedstocks coupled with effective production processes are required (Bazzanella et al., 2017; Zimmerman et al., 2020). This approach could remove the need for fossil fuels entirely, significantly decreasing the global warming potential (GWP) of the chemical industry, however significant amounts of renewable energy are required (Kätelhön et al., 2019). There is an increasing and urgent need for sustainability in the chemicals industry, by both material reuse and emission reductions: companies such as SABIC and Unilever aim to eliminate fossil fuel feedstocks from certain products as early as 2030 (SABIC, 2020; Unilever, 2020; Cefic, 2021). Meanwhile, a number of start up companies aim to use only waste as feedstock, for example BioBTX (2020) and Lanzatech (2021).

All renewable benzene production routes are technologically immature and there is a limited understanding of relative sustainability and viability. This is especially true for benzene over other aromatics, therefore the objective of this assessment is to ascertain the most promising routes, whilst identifying key areas of research, impact and technology hotspots. No review has yet been conducted into the relative sustainability of synthetic benzene production routes. While detailed Life Cycle Assessment (LCA) and Techno-Economic Analysis (TEA) are not yet possible for many of the low technology readiness level (TRL) routes above, a screening is important to understand and direct research veins

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Nomenclature

(H)ZSM-5	(Hydrogen) Zeolite Socony Mobil-5
3P(s)	'People', 'Profit' and 'Planet'
AHP	Analytical Hierarchy Process
BTX	Benzene, Toluene, Xylene
CAPEX	Capital Expenditure
CDU	Carbon Dioxide Utilisation
CLD	Chemical Liquid Deposition
CMA	Catalytic Methane Aromatisation
EPA	Eicosapentaenoic acid
FT	Fischer-Tropsch
GWP	Global Warming Potential
LCA	Life Cycle Assessment
MCDA	Multi-Criteria Decision Analysis
MTA	Methanol to Aromatics
NGO	Non-Governmental Organisation
OPEX	Operational Expenditure
PCC	Pearson Correlation Coefficient
SCO	Single Celled Organism
SDG	Sustainability Development Goal
STA	Syngas to Aromatics
TEA	Techno-Economic Analysis
TEOS	Tetraethoxysilane
TRL	Technology Readiness Level
WHSV	Weight Hourly Space Velocity

and inform policy makers, given the widespread use of benzene. A comparison to traditional production from non-renewable crude oil is considered out of scope for this assessment as is fundamentally unsustainable (Wunderlich et al., 2021).

2. Literature review

There are many potential synthesis routes to benzene, each with advantages and disadvantages. The carbon source either can be biogenic, CO_2 or other wastes Fig. 2.1. Many routes produce a range of aromatic products and therefore can be considered as part of a wider 'refinery' that is not limited to benzene, but values each product. Toluene, xylenes and various derivatives are currently produced in similar refinery processes to benzene and transition to renewable synthesis would incur similar sustainability benefits to that from benzene.

2.1. Routes from Syngas to Aromatics (STA)

Syngas is a mixture of primarily CO and H_2. Syngas can be produced from fossil fuels, biomass or gasification of wastes (Wilhelm et al., 2001). Early aromatic synthesis routes include syngas based Fischer-Tropsch (FT) processes. However, FT produces an Anderson-Schulz-Flory distribution of mostly linear hydrocarbons and coupling with HZSM-5 for conversion aromatics, results in aromatics selectivity of only <50%, due to unfavourable low reaction temperatures (Zhou et al., 2019). This is especially true for benzene, requiring higher reaction temperatures for demethylation (Zhu et al., 2013). This has been overcome by Wang et al. (2014) (Route 1)[1] using Fe/Fe_3O_4 nanoparticles, achieving an exceptionally high benzene selectivity of 48%. Unfortunately, CO conversion rate is not specified and the technology is in its infancy (TRL 3).

'One-pot' syngas to aromatics routes have become preferable in research due to their simplicity and high selectivity for aromatics, but at the expense of benzene selectivity. These are typically use a methanol, dimethyl ether or olefin intermediate. For example, Cheng et al. (2017), used Zn-ZrO_2 nanoparticles dispersed on HZSM-5 with multiple TEOS CLD cycles to achieve20% CO conversion and 50% selectivity for BTX (Route 2). Notable here was the increase in catalyst stability, seeing no degradation over 1000 h with consistent productivity of 0.12 g/gcat hr. Zhou et al. (2019) were able to improve CO conversion and specified benzene selectivity (Route 3). Mo-ZrO_2 nanoparticles were instead used, but catalyst degradation was an issue after only 100 h due to Mo leaching. One novel advancement was the use of high pressure H_2 to avoid coking, hence improve yield. Miao et al. (2020) were able to improve benzene selectivity with an MnCr-ZSM-5 catalyst, stable over the 100 h test period (Route 4). The addition of a secondary catalyst bed of ultra-stable Y zeolite (USY), contributed to benzene selectivity, although the CO conversion was lower. While direct STA routes have low benzene selectivity, no study had the explicit goal of making only benzene, instead a range of aromatics. As all are low TRL (3), further work may improve selectivity and each offer novel ways to improve production.

Certain biomass-based routes use a syngas intermediate before conversion to aromatics. BioBTX (2020), a Netherlands based company, aims to commercialise a TRL 6 patented process involving biomass or waste plastic pyrolysis before STA (Route 5). Viability stems from recycling heavier pyrolysis products and co-feeding alongside biomass to increase conversion and selectivity. Niziolek et al. (2016a, 2016b) described in detail how biomass-based BTX production might be implemented, outlining specific industrial synthesis routes whilst comparing different biorefinery orientations. The most profitable refinery (Route 6) utilises a hardwood biomass (similar to Route 8) due to its low cost; found to have the most profitability influence. After gasification, STA proceeds via a water gas shift reaction, methanol synthesis and finally methanol to aromatics (MTA). The Ag/HZSM-5 catalyst is given little thought, providing scope for improved benzene yield. Niziolek et al. (2016a, 2016b) highlighted the difficulty and expense in use of biomass compared to fossil-based syngas and possibly CO_2 via the extensive preprocessing steps that add significant capital cost. Despite this, the most profitable refinery modelled has net present value of $1.2 billion and a payback time of 9 years. Also, the plant represents an emissions reduction of 80–85% relative to fossil alternatives. VTT, a Finland based research centre, has developed a process to gasify woody biomass, convert to hydrocarbon using FT before aromatisation over Zn and La doped HZSM-5 (Reinikainen et al., 2015) (Route 8). The process has reached the end of lab scale testing and is ready to be further scaled (TRL 4). Selectivity at highest profitability gives 7% benzene, while at lower profitability, 18% is possible. VTT estimates an overall cost of 1.4 €/l of hydrocarbon product over a 20 year plant lifespan (Chemical Processing, 2015).

Niziolek et al. (2016a) alternatively proposed conversion of methane to aromatics via syngas and methanol intermediates (Route 7). The process incorporates the Reverse Water-Gas Shift reaction (RWGS) to further convert process generated CO_2, hence may also be a viable method for biogas conversion. LPG produced during methanol conversion can be upgraded to aromatics (dependant on market pricing) using the Sabic-owned Cyclar process, leaving the only major products as O-xylene, benzene and water. Economics and energy use are investigated, again finding scale determines viability. Benzene selectivity could be tuned, with the catalyst again given little thought.

2.2. Biomass based (non-syngas)

Aromatics can be derived by catalytic depolymerisation of lignin using HZSM-5. Fan et al. (2014) produced benzene at 4.5% yield (9). Zhu et al. (2013) instead first converted lignin to bio-oil before catalytic cracking, demonstrating an overall 3% benzene yield from biomass (Route 10). Zhu, Wang and Li also demonstrated the importance of low weight hourly space velocity (WHSV)[2] on benzene production specifically, requiring further exposure to catalyst and heat for removal of

[1] Each route has been given an identifying 'route number' shown in bold type at the end of each route description and are used for identification throughout the study.

[2] Weight hourly space velocity (h^{-1}) is the mass flowrate of the feed divided by mass of catalyst i.e. a low WHSV indicates a high residence time for a given mass of feed relative to the mass of catalyst.

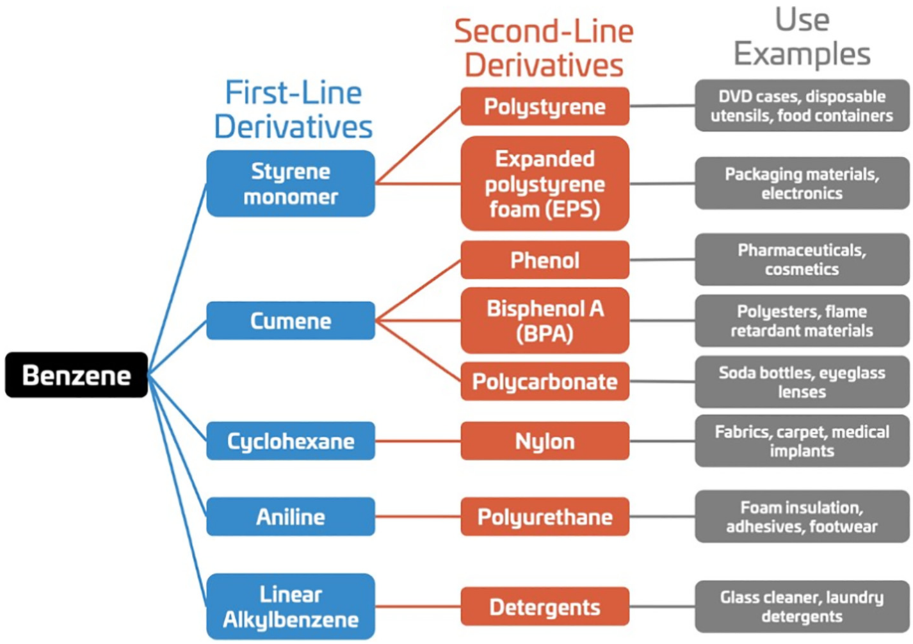

Fig. 1.1. Benzene and its derivatives.

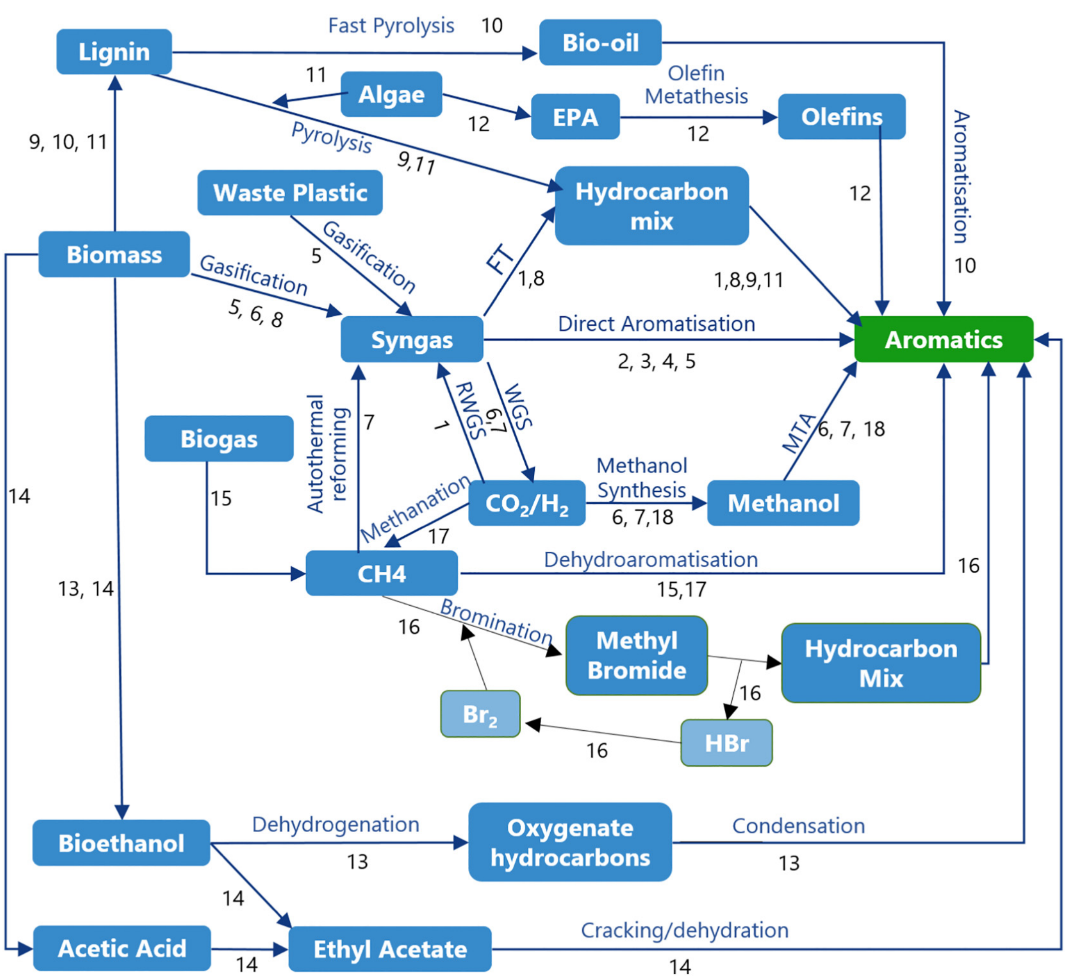

Fig. 2.1. Routes to Aromatics (each route is numbered).

groups: benzene yield doubled between 3 h^{-1} and 1 h^{-1}. The fast pyrolysis of lignin to, and subsequent cracking of bio-oil has been patented in the US by Anellotech (2019) (see also Sorenson (2017)), showing a higher TRL of 6. However, this process only produces 20% aromatics and does not specify benzene, hence it is excluded from this analysis.

Wang and Brown (2013) developed a conversion route to aromatics via pyrolysis using algal single celled organisms (SCO) (Route 11). However, benzene selectivity was low (5% of carbon yield) despite the high temperature and detail is limited. This route advantageously produces ammonia, then used as fertilizer to grow additional feedstock. Biomass based studies involving pyrolysis and subsequent aromatisation were typically conducted prior to the latest developments in relevant catalysis, hence the low conversions and selectivities. Huang et al. (2013) and Pingen et al. (2018) have developed procedures for converting specifically algae SCO or yeast derived eicosapentaenoic acid (EPA) into benzene, with exceptionally high conversion and benzene selectivity (Route 12). This one-pot process forms a 1,4-cyclohexadiene intermediate through olefin metathesis before dehydrogenation to benzene. However, the EPA feedstock is currently prohibitively expensive.

Virent, a Wisconsin based company, alongside Johnson Matthey, have developed a near-commercial route named 'Bioforming' (Held et al., 2014; Virent Inc, 2021). Commercial p-xylene production with BP (2019) is being pursued. The technology is broad, aiming to produce a number of hydrocarbon products used in both fuels and chemicals via a variety of pretreatments and catalysts. 3 patents focus on improving the aromatics yield: from carboxylic acid feed (70.7%) (Blommel and Cortright, 2014), di/poly- oxygenate feed (63%) (Beck et al., 2014) and, at best, from alkanols (73%) (Route 13) ((Blommel et al., 2015), see example 13)). Unfortunately, none specify benzene yield or selectivity. The highest aromatics yielding route given in example uses an ethanol feed and copper-zinc-alumina and nickel-nitrate ZSM-5 catalysts.

Dedov et al. (2020) investigated the novel conversion of ethyl acetate to BTX over H-MFI resulting in 25% BTX selectivity, although benzene was not specified and C2+ hydrocarbons are theoretically limited to 64% (Route 14). Ethyl acetate can be produced renewably from bioethanol and acetic acid, but the expense relative to raw biomass feedstocks reduces viability.

2.3. Biogas based

Galadima and Muraza (2019) conducted a recent literature review on Catalytic Methane Aromatisation (CMA) (renewable when using biogas). This one step process is similar to that of syngas; the most effective methods use the same Mo/ZSM-5 catalysts. Nano-catalysts were shown to be more stable and active. Novel work involving GaN catalysts was highlighted but will not be discussed here due to technological immaturity. Investigating catalyst preparation techniques, Velebná et al. (2015) found microwave irradiation assisted wet impregnation best (in contrast to Kasipandi and Bae (2019)), achieving high conversion and selectivity, although catalyst degradation was an issue (Route 15). GTC Technologies have developed an alternative route, activating methane using bromine (Route 16). Although patented, claimed to be ready for scale and economically viable with high conversion, no further references have been found (DuBose, 2015). Methane based routes typically use pure methane in laboratory experiments, and it is unknown if similar performance would be observed when using biogas; usually containing high CO_2 and contaminant gases. Although, as shown below, it seems likely CO_2 would also convert to hydrocarbon.

2.4. Tandem catalysis and the explicit use of CO_2

Zhu et al. (2017) coupled methanation of CO_2 with CMA in 'tandem catalysis', although in separate reactors; methanation using Ni/SiO2 and subsequent dehydroaromatisation with Mo/HZSM-5 (Route 17). Despite low methane conversion, high benzene selectivity was achieved, hence the route is promising if an effective recycle could be utilised. The novelty of these routes is in the use of CO_2 to aid emission reductions and, in comparison to methane, the cheaper feedstock may offset the higher cost of a second reactor. Prior studies by Wang et al. (2000) and Shu et al. (2002) highlighted the use of high pressure CO/CO_2 in the aromatisation atmosphere to suppress coke formation and enhance benzene formation. This has also been used to utilise a methanol intermediate in a single reactor with a bifunctional catalyst (Zhang et al., 2019; Wang et al., 2019) (Routes 18, 19). At best, this has achieved a BTX fraction of 44% although, as combining exothermal methanol synthesis with high temperature aromatics formation is thermodynamically unfavourable, benzene selectivity is much lower. Given the ease of this method, it may be viable to pass the aromatics to a second, higher temperature reactor to produce more benzene, although defeating the single reactor objective.

In summary, there is a global need for sustainable production of chemicals (including benzene), de-coupling the industry from fossil fuels. This challenge primarily involves finding suitable alternative carbon feedstocks and efficient catalysts. The energy requirements are immense, hence research outputs need to consider economic and operational realities of industry and, to be worthwhile, renewable energy must be used. It is unlikely that benzene would be produced alone, given the incentives for p-xylene and the low benzene selectivity of all routes. Most routes have interchangeable aspects e.g. syngas can be produced from waste plastic or biomass before following the same conversion route and notably use variants of ZSM-5. So, it seems unlikely that any one independent route would be optimal, instead the successes from each used in combination. Further analysis of the routes through MCDA will aim to identify and highlight those successes and research areas worth pursuing.

3. Assessment methods

Sustainability is defined as using resources and processes so not to deplete that available for, or harm, future generations (Azapagic and Perdan, 2000). The United Nations 17 'Sustainability Development Goals' (SDGs), call for action to ensure sustainable economic and social development (United Nations, 2015). The SDGs serve to highlight the importance of solutions that address the three pillars of sustainability; 'People', 'Profit', 'Planet' (also known as 3Ps) and do not neglect, for example, societal issues for environmental benefit or safety for economic performance. Hence, these categories are used as a basis for assessment. Depending on the context and preference of institutions, companies or individuals, various quantitative and qualitative KPIs may be more/less important, but are nevertheless all relevant and form an indicator framework for assessment purposes.

Within sustainability assessment, once an indicator framework has been developed, appropriate weightings can be assigned to each indicator dependent to the specific scenario or case study. Multiple Criteria Decision Analysis (MCDA) is often used to achieve this (Velasquez and Hester, 2013). MCDA encompasses a range of specific techniques of varying complexity. Almost all begin with 'quantitative elimination' to discard obviously inferior alternatives, before assigning each a score per indicator and applying weighting or allowing competition within a model. The outcome is an informed and balanced ranking or comparison of alternatives to aid the decision maker.

Here, assessment was conducted in three steps, firstly to reduce the less viable alternatives and narrow the field of comparison, secondly to conduct the screening (MCDA) and thirdly to evaluate the sensitivity and uncertainty of the results (Fig. 3.1).

3.1. Step 1: pre-screening elimination

Screening of alternatives first requires an elimination of inferior routes, before those selected are evaluated in further detail, then applying performance scores against indicators through MCDA. Usually for deployment feasibility studies, elimination can be quantitative and is

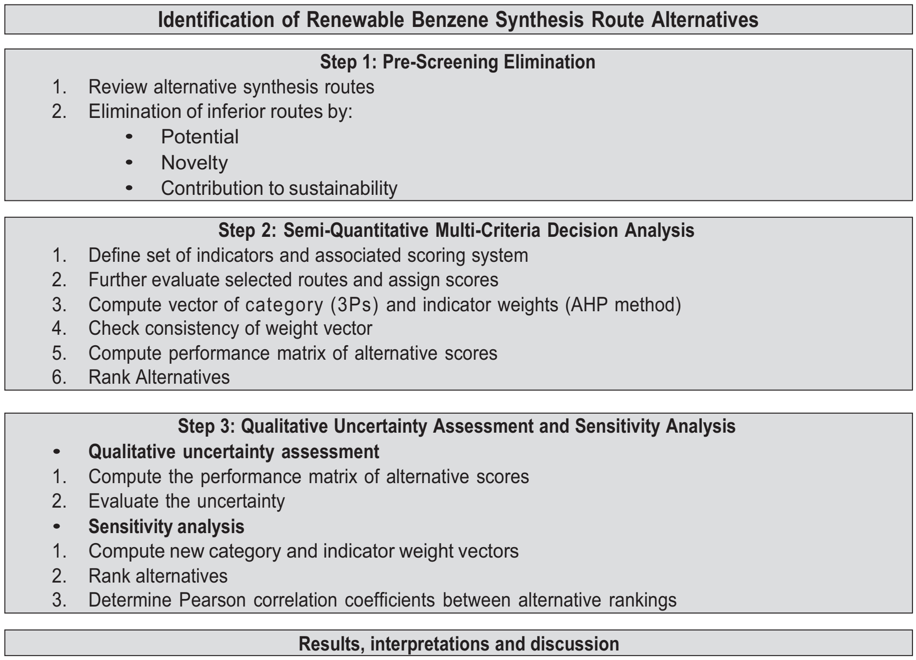

Fig. 3.1. Assessment framework, adapted from Chauvy et al. (2019).

most commonly based on TRL. Given the similar immaturity (TRL 3–6) of all benzene routes, those retained instead demonstrate potential, novelty and contribution to sustainability across both qualitative and quantitative areas. Table 1 summarises the nine retained routes. Route 1 (CO_2/syngas based) offers a unique avenue of research as the only route (with sufficient information) not using a zeolite based catalyst. Also, despite its low maturity, benzene yield was high. Of the one-pot STA routes, Route 2 was chosen for low catalyst degradation, with similar aromatics yield to Route 3. Operation temperature and pressure is lower, hence likely lower OPEX cost. Despite the use of USY in Route 4 to roughly double the benzene selectivity, the reduced conversion provides a similar overall yield, hence was eliminated.

Both biomass-based STA routes proposed by Niziolek et al. (6 & 7) had well developed technical and economic information. Route 7 was chosen over Route 6 due to higher conversion, benzene selectivity and CO_2 integration, hence potential to use biogas. Despite the claim of commercial viability, Route 5 (BioBTX) does not specify the catalyst, feedstock or process to achieve an average benzene yield and yielding any analysis difficult. And, although the only route to explicitly use plastic, any syngas or CO_2 based route in theory is also capable. By contrast, the ready-for-scale Route 8 (VTT) provides ample detail and options for a high benzene yield or maximised overall profit, depending on manufacturer/market preference. Similarly, Route 13 is close to commercialisation using available catalysts and with high aromatics selectivity via a unique process.

The two lignin based routes (9 & 10) are numerically very similar (operating conditions, conversion, selectivity), but intermediate use of bio-oil is not worthwhile, as Route 9 gives higher benzene yield by a simpler one-pot process. Route 12 has been eliminated despite unmatched conversion and selectivity from EPA, as cost is prohibitive. Route 11 is uniquely able to grow more feedstock using the ammonia by-product. Route 14 has been eliminated as although unique in use of ethyl acetate, its extensive production from base feedstocks via bioethanol and acetic acid is unlikely to be energetically or economically favourable compared to other routes.

In a comparison of the biogas to aromatics routes, the purportedly ready-for-scale Route 16 (GTC) has been eliminated due to a lack of information. Route 15 has been retained primarily due to high selectivity, but also to represent the use of biogas, given the potential for combination of MTA and CDU technologies. The reviewed CDU routes (17, 18, 19) have been developed as part of ongoing research by the same group and hence use the same base technology. While each was worthwhile of review due to notable differences in catalyst and method, only Route 18 is selected. Although 17 has the highest yield, side products are low value C1 and C2 gases, so viewed as part of an overall refinery, preference for more valuable aromatic side products coupled with the simpler, continuous, one-pot process make 18 the more realistic industrial choice. Route 19 has lower conversion and greater catalyst degradation.

Note that while technologies may have been eliminated at this stage, this is no indication to halt research and development, as may be useful or superior in future under changed circumstances. For example, Route 12. If currently prohibitive EPA costs are overcome by industrialised production via algae (rather than fish oil) as suggested by Wang et al. (2014), it represents the most selective and efficient route for benzene specifically, avoiding almost all side products.

3.2. Step 2: semi-quantitative multi-criteria decision analysis

Indicators were selected and grouped into categories of either 'People', 'Profit' or 'Planet', allowing for subsequent additional weighting and to show alignment with core sustainability principles as outlined by United Nations, (no date) and Edenhofer et al. (2012). Indicators chosen specifically focus on the process rather than unknown organisational or deployment scenarios. This is particularly applicable for 'People' (social) based indicators where 'employment or labour' based indicators cannot be determined at this stage. The full scoring guide (Table S1) and information sources can be found in the Supporting Information. Assigned scores and justification can be found in the included Excel workbook.

3.2.1. Indicators

3.2.1.1. People indicator 1: potential for supply chain discriminatory practices. While it is likely any new technology will be deployed in wealthier countries first, many of the components originate in developing countries and supply chain analysis will include these. This indicator amalgamates ideas used by McCord et al. (2021) including equal

Table 1
Selected routes to non-fossil benzene.

Route	1	2	7	8	9	11	13	15	18
Technology in Brief	STA (indirect)	STA (direct)	CH4 > Syngas > methanol > aromatics	Gasification > FT > aromatisation	Biomass (lignin)	Biomass (algae)	Biomass	Gas to aromatics	Tandem catalysis of CO_2
References	(Wang et al., 2014)	(Cheng et al., 2017)	(Niziolek et al., 2016a)	(Reinikainen et al., 2015)	(Fan et al., 2014)	(Wang and Brown, 2013)	(Blommel et al., 2015): Example 13	(Velebná et al., 2015)	(Wang et al., 2019)
Feed	CO_2/H_2 1:1	Syngas H_2/CO 2:1	Methane	Woody biomass converted to syngas (H_2/CO 7:5)	Lignin	Algae (SCO) *Chlorella vulgaris*	Biomass (bioethanol)	Methane	CO_2/H_2 3:1
Catalyst(s)	Fe/Fe_3O_4 nanoparticles	Zn-ZrO_2 nanoparticles HZSM-5	MTA: Ag/ZSM-5 LPG to aromatics: Ga/ZSM-5	FT: Fe base w/ Si, Cu, K Aromatisation: HZSM-5 w/ Zn & La	HZSM-5	HZSM-5	Dehydrogenation: Cu-Zn-Aluminate (commercially available as Shiftmax 230) Condensation: Nickel nitrate on ZSM-5	Mo/ZSM-5	Cr2O3 nanoparticles HZSM-5
Passivation (cycles)	N/A	TEOS (2 cycles)	Not specified	Not specified	Not specified	Not specified	ShiftMax230 is 11% Al2O3 ZSM-5 is Al2O3 bound (20%)	Not specified	Silicalite 1
Metal (or oxide)/zeolite ratio	N/A	1:2	Not specified	0.6% Zn, 0.8% La	N/A	N/A	ShiftMax 230 - N/A Ni loading 1%	Not specified	1:1 mass ratio
Feed/catalyst ratio	Not specified	Not specified	Not specified	Not specified	1:2	Not specified	0.8 h^{-1} WHSV	Not specified	1:1
Operating conditions	1 atm/520 °C	3 MPa/380 °C	Autothermal reforming: 1000 °C, 30 bar RWGS: 400 °C, 26 bar Methanol Synthesis: 250 °C, 45 bar MTA: 425 °C	Gasifcation: 800 °C FT: 300 °C/0.5 MPa Aromatisation: 400 °C/0.1 MPa	1 atm/550 °C	1 atm/800 °C/	Dehydrogenation: vary from 25 °C to 370 °C, 20.7 bar Condensation: 25 to 350 °C, 6.9 bar	1 atm/700 °C	3 MPa/350 °C
Continuous/batch	Batch (40 min)	Continuous	Not specified	Not specified	Continuous	Not specified	Semi-Batch	Continuous	Continuous
Conversion (mol%)	Not specified	20% CO to HC	66%	Not specified	25.3% C to BTX 90.1% C to HC	24 mol% C to aromatic HC	75% C to HC	14.8% CH4 to aromatics	34% CO_2 to aromatics
Benzene selectivity/yield	48 mol%	Not specified	8.2% of C yield	18 wt% best 7 wt% at most profitable	5 mol% of C	5 mol% of C	Not specified	80 mol% from CH4	0.9% from CO_2
Other significant products (selectivity)	Butane (0.14) Aromatics (0.77)	Aromatics (0.8) BTX in aromatics (0.63)	O-xylene (0.58), water	Aromatics (0.8 at best, 0.49 w/ high benzene)	BTX (0.253 of C)	Aromatics (0.24 of C)	Aromatics (0.97)	Toluenes Xylenes C9 aromates Napthalene	Aromatics (0.76 total) BTX (0.436) P-Xylene (0.253)
TRL	3	3	4	4	3	3	6	3	3
General mechanism	One-pot, RWGS FT boudward reaction stepwise addition reduction trimerisation keto-enol tautomerisation reduction stepwise demethanation	One-pot, methanol intermediate	Autothermal reforming: CH4 to syngas RWGS: syngas cleaning + CO_2 conversion Methanol Synthesis MTA LPG to aromatics (Cyclar - Sabic)	Gasification FT Aromatisation	One-pot, Pyrolysis Aromatisation	Pyrolysis Aromatisation	Biomass pretreatment (fermentation) to ethanol Dehydrogenation Condensation (3 reactors for ethanol to aromatic steps)	Dehydroaromatisation	Methanol synthesis (formate route) MTA
Zeolite Si/Al ratio	N/A	120	Not specified	Not specified	25	23	Not specified	20.4	40
Catalyst lifetime	Not specified	>1000 h	Not specified	Not specified	Limited information (3 runs)	Not specified	Not specified	Conversion drop from 14.8% at 60 min to 9% at 240 min	>100 h
Route novelty	High benzene selectivity	Catalyst stability One step	Uses all components of biogas, detailed economic analysis, combines CO_2 and methane use	Commercially viable, Economic estimations given	Actually uses biomass, One step	Use of algae directly, also produces ammonia for fertilizer	Use of commercially available catalysts High TRL with investment from large companies within industry high aromatics selectivity	Use of methane High selectivity	1 pot Use of CO_2 Use of CO_2 reaction atmosphere

opportunities in labour, potential for exploitation and child labour, and conflicts or corruption in supplying countries. Emphasis is placed on the conflict mineral component(s) of the catalyst as other components are more widely sourced (biomass, biogas etc.). ZSM-5 supply is largely ignored as does not differentiate routes, used in all except route 1.

3.2.1.2. People indicator 2: health & safety. Often risks during chemical manufacture are inherent; able to be mitigated but not eliminated and therefore it is important to prevent the development of dangerous technologies before maturity. This indicator aims to account for both occupational hazards during production and risk to the surrounding community, should loss of containment occur. Scale is based on number and severity of identified risks, and the potential impact to external communities. While benzene emission would be hazardous as a known carcinogen, this would only occur in a loss of containment scenario due to operational error unrelated to the base technology. Hence, it is not included in the assessment, although it can be noted that benzene emission is inherently less likely for more simplistic routes.

3.2.1.3. Profit indicator 3: carbon efficiency (yield). The conversion efficiency from base feedstock to benzene may be better illustrated via a carbon yield than mass yield as some feedstocks will have many non-useful components (e.g. lignin) while others will not (e.g. methane). Many routes begin with a product of pre-treatment, assuming prior processing, for example, Virent's direct use of bioethanol without pre-processing (Route 13). Pre-treatment/processing is not standardised and in some cases the base feedstock can be debated, e.g. should air be considered the base feedstock instead of captured CO_2? Hence, carbon efficiency (yield) over the main reaction stages is used, in accordance with most literature. While product purity (and hence degree of required separation) will in part be a function of carbon efficiency, separation is excluded from the assessment due to lack of available information given the low technological maturity of most routes. Where not specified in literature, calculations are given in relevant supporting information table (Section 6).

3.2.1.4. Profit indicator 4: geographical constraints. Widespread technology adoption depends partially on geographical constraints (e.g. inhibitive land cost for large scale plants or feedstock availability variation). This account indicator accounts for crustal abundance, reserve distribution, production concentration, recycling rate and political stability of a particular element. Higher supply risk also indicates higher transportation costs.

3.2.1.5. Profit indicator 5: economic feasibility. As most of the routes are low TRL little information is available regarding scale up economics or feasibility. Hence, it is not useful to attempt to quantify indicators such as relative added value or net present value. Instead, a range of factors is used, including wider literature opinion and information availability, commercial interest/involvement, exposure to price fluctuations (excluding benzene), energy requirements and simplified relative added value calculations (feed vs product values). Although OPEX is expected to be more influential, relative CAPEX will also be considered. Hydrogen is expected to be a significant cost (Amos, 1998). No routes are expected to be competitive to standard benzene production and so no comparison is made at this stage. Details on cost calculations can be found in Supporting Information Section 3.

3.2.1.6. Profit indicator 6: energy requirement. While Economic Feasibility incorporates renewable energy requirements, it is important to separate and highlight as an indicator due to the frequent citations as a limiting factor to a sustainable future, free of fossil fuels. It is assumed all energy is sourced renewably (and not from fossil fuels) hence 'Energy requirement' is not directly linked to 'Emissions Reduction Potential'. Due to low TRL and lack of information, it is impossible to accurately determine industrial, qualitative energy requirements; usually found via modelling and simulation. Screening studies often use reaction enthalpy changes as proxy, but due to the complexity and unknown product ratios of reactions here (e.g. Fischer-Tropsch), this is not possible. Hence, a semi- quantitative scale is used, including numerical temperatures and pressures in addition to qualitative factors such as requirement for energy intensive biomass pre-treatment. Catalyst production is included as significant amounts are used (typically ratios around 1:1 with feedstock). The highest energy requirement will likely come from separation but, as all routes produce a variety of hydrocarbons and none have a majority benzene product (hence requiring similar degrees of separation), this is not used to differentiate and is beyond the scope of this study.

3.2.1.7. Planet indicator 7: environmental performance. A broad indicator that qualitatively highlights various environmental effects (negative or positive), typical of LCAs and was outlined by Azapagic and Perdan (2000). Here, Global warming potential (GWP) is excluded as is included in Emission Reduction Potential.

3.2.1.8. Planet indicator 8: emissions reduction potential. Primarily determined via 100-year Global Warming Potential (GWP 100a) values. While it is impractical to conduct a detailed GWP balance at this stage, magnitude estimates highlight significant benefits/issues of uptake and mitigation. Assumptions and calculation examples can be found in Supporting Information Section 4.

3.2.1.9. Planet indicator 9: TRL. Technology readiness level (TRL) is widely used to consider technology maturity (U.S. Department of Energy, 2011). The scale considers confirmation of principles, literature, prototyping scale (lab/pilot/full), and feed flow testing.

3.2.2. Scenarios, indicator and 3P weighting

When evaluating routes, example scenarios can be utilised to create artificial decisions and justify 3P and indicator weighting choices in non-specific, real world scenarios (Cremonese et al., 2020). All scenarios assume adequate market demand for renewable benzene. As the scenarios used are theoretical, an adaptable spreadsheet tool[3] has been developed to allow assessors to assign alternative weightings based on. Three scenarios are exemplified:

Scenario 1: Multi-National Corporation in Developed Country.
Scenario 2: Start-up in Developing World.
Scenario 3: Research Institution.

Full descriptions of the goals and motivations used in each scenario can be found in the Supporting Information Section 2.

Weight sets were developed for both the 3Ps and indicators using the Analytical Hierarchy Process (AHP) as developed by Saaty (2008). Each category or indicator undergoes pairwise comparison using linear scales based on perceived stakeholder preference per scenario. Scores are compiled in a pairwise comparison matrix as shown below. While the 3Ps have only been weighted using 3-point comparison (Ternary AHP), more granularity was required for indicators, instead using a 9-point scale (detailed in supporting information Section 7). Scores are compiled in an n x n pairwise comparison matrix, where n is the number of 3Ps or indicators. Entry bjk describes the relative importance of indicator/3P j to indicator/3P k.

$$B = \begin{bmatrix} 1 & b_{12} \cdots & b_{1n} \\ b_{21} & 1 \;\ldots & b_{2n} \\ \vdots & \vdots \;\ddots & \vdots \\ b_{1n} & b_{n2} \cdots & 1 \end{bmatrix}$$

[3] Adaptable spreadsheet tool is available as a separate Excel file. Specific circumstance or in response to further technological development.

Weight vectors w are computed for each comparison matrix, with weighting wj for each row:

$$w_j = \frac{\sqrt[n]{\prod_{j=1}^{n} b_{jk}}}{\sum_{j=1}^{n} \sqrt[n]{\prod_{j=1}^{n} b_{jk}}} \quad (1)$$

To compute the final scores for each indicator per scenario, each score aij (indicator j score per alternative route i) in the unweighted performance matrix A is multiplied by both 3P and indicator weights (Eq. (2)) to produce the final double weighted performance matrices.

$$A = \begin{bmatrix} 1 & a_{12} \cdots & a_{1n} \\ a_{21} & 1 \quad \ldots & a_{2n} \\ \vdots & \vdots \quad \ddots & \vdots \\ a_{1n} & a_{n2} \cdots & 1 \end{bmatrix}$$

$$\textit{Double weighted score}, s_{ij} = w_j^{3P} w_j^{ind} a_{ij} \quad (2)$$

Scores per alternative route i are totaled to produce a final ranking of route suitability per scenario, where the highest score indicates the most preferable route.

3.2.3. Weight vector consistency check

A consistency check is performed as part of AHP to ensure consistency between indicators within a matrix i.e. many instances of extreme values within a single matrix (e.g. 0.14, 7) indicates low consistency for the given 3P.

3.3. Step 3: qualitative uncertainty assessment and sensitivity analysis

3.3.1. Qualitative uncertainty assessment

An uncertainty performance matrix was constructed in addition to the primary performance matrix, evaluating each of the 3Ps against 3 indicators: System Representativeness, Reliability of Source and Validation, Completeness. This broadly follows the methodology given by Chauvy et al. (2019). The scores were normalised to a percentage (Eq. (3)) before uncertainty values were calculated using the same 3P weighting as previous (Eq. (4)).

$$\bar{a}_{ij} = \frac{a_{ij}}{4} \quad (3)$$

$$\textit{For } i = 1, 2, \ldots, M \textit{ and } j = 1, 2, \ldots, N$$

$$u(a_i) = \sum_{i}^{j} \bar{a}_{ij} w^{3P} \quad (4)$$

$$\textit{For } i = 1, 2, \ldots, M \textit{ and } j = 1, 2, 3$$

3.3.2. Sensitivity analysis

The AHP scores are assigned by the assessor and although based on case studies without bias, subjectivity will inevitably influence scoring. This effect is minimised in final ranking as offers lower granularity. To assess this influence, new weight vectors were computed, altering original weights by ±5%, ±25%, and ± 50% for each ‘P’ to provide the new ranking outcome. New ranks were compared to both reference scenario 1 and alternative new rankings using a Pearson Correlation Coefficient (Eq. (5)), again in pairwise comparison.

$$r = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{\left[n\sum x^2 - (\sum x)^2\right]\left[n\sum y^2 - (\sum y)^2\right]}} \quad (5)$$

4. Results and discussion

4.1. Unweighted results

Within the unweighted results (Table 2; additionally, full detailed results can be found in the Supporting Information Section 6), Routes 1 and 9 performed the strongest across the sustainability indicators. Route 1 coupled the use of an Fe/Fe_3O_4 nanoparticle catalyst with CO_2/H_2 feed to produce benzene, while Route 9 pyrolyses a lignin feed in the presence of HZSM-5 to achieve subsequent aromatisation of the gases. Route 9 uses no metals, beneficial for Environmental Performance indicators, due to negating the need to mine. Route 1 benefits from a significantly higher carbon efficiency than any route and generally low energy requirement, arising from simplicity in a one-pot process and little

Table 2
Unweighted performance matrix.

3P	Indicator	Route 1	2	7	8	9	11	13	15	18
People	Health & Safety	3	1	1	1	3	1	1	1	1
	Potential for Supply Chain Discriminatory Practices	2	2	1	0	4	4	0	1	1
Profit	Carbon Efficiency	4	1	2	1	1	1	1	2	0
	Geographical Constraints	1	1	0	0	4	2	1	0	1
	Economic Feasibility	2	2	3	4	1	1	4	2	2
	Energy Requirement	3	1	1	1	2	2	0	2	3
Planet	Emissions Reduction Potential	2	2	1	2	3	1	1	3	2
	Environmental Performance	2	2	2	1	1	3	1	2	2
	TRL	1	1	2	2	1	1	4	1	1
	Total per route	19	12	11	10	19	15	9	13	12
	Route Rank	1	4	5	6	1	2	7	3	4

A colour gradient is used as a visual aid to indicate relative scoring. Each colour represents a score i.e. 0 (red) is the worst score a route could achieve for a given indicator, while 4 (dark green) is the best.

feed pre-treatment requirement. Both routes led on 'People', with scores (19) significantly higher than any other route (9–15).

4.1.1. Wide influences: catalysts & technology maturity

Catalysts influenced all indicators to varying magnitudes, therefore, are identified as a hotspot. Determined by the scoring scale, the influence ranged from direct and strong, such as for Potential for Supply Chain Discriminatory Practices, to indirect and weak as for Energy Requirement. Where catalyst requirements were uncertain, routes generally scored worse. This was notable for Route 7 which while well developed in other areas (economics, TRL), fell short in both Health and Safety and Emissions Reduction Potential due to uncertainty around catalyst volume requirement. Catalyst type and lifetime were also route differentiators. Future focus towards particular catalyst technologies will have a strong influence on the most preferred routes. Catalyst regeneration was not accounted for due to the low maturity of the catalysts and hence lack of performance metrics in an industrial context. However, given the wide reaching impacts, this would have a significant influence on final rankings. Route 2 is highlighted for its exceptional catalyst lifetime with no deactivation over 1000 h, coupled with reasonably good selectivity.

Technological maturity did not directly differentiate routes, although did have a strong indirect influence on numerous indicators. Often less mature routes showed more promise in other areas, such as carbon yield (Route 1) or the aforementioned catalyst stability (Route 2). The high maturity Route 13 (TRL 6, scoring 4) serves to further prove this point, scoring the lowest total overall. This was largely due to a high level of data uncertainty from qualitative sources such as patents or press releases. For example, the exact catalyst and resulting carbon yield were not specified or determinable. Further correlation with high maturity was high Energy Requirement (scoring low) for both Routes 7 and 13, but this may be due to more developed, complex routes realising more energy requirements, rather than a reflection of the individual technology.

4.1.2. People indicators

Routes generally scored 1 for Health and Safety (i.e. many sources of potential harm have been identified and would require controls. Potential risk to surrounding community), although no serious risk to the community was identified in any route. This may be conservative, although many areas are uncertain at this stage. In particular, the exposure risk from nanoparticles is not well known and may vary with elements used due to the similar size to biological molecules (Aitken et al., 2004). Where nanoparticles are not used, many risks still arise from the use of metal powders in catalysts, high temperature and pressure risks are inherent in many routes, although minimised through optimisation. Potential for Supply Chain Discrimination instead ranged considerably from 0 (Routes 8 and 13) to 4 (Routes 9 and 11). Those routes scoring poorly generally showed potential for corruption, child labour (specifically in Chile, Indonesia and Kazakhstan) and connections to Russia or China, home to ongoing conflicts. The gender gap was not a differentiating issue, all routes scoring 'low' to 'medium' with the exception of India (high – Route 18,).

4.1.3. Profit indicators

Carbon Efficiency ranged significantly from 0.23% (Route 18) to 49% (Route 1), although most varied from 5% to 15%, revealing an area for necessary development. This may be an unfair assessment however, as many routes did not have the explicit goal of benzene production, rather aromatics generally, with a preference for p-xylene. Route 1 had significantly higher Carbon Efficiency than Route 7 at 12.3% in 2nd position, a major factor to its overall success. Notably, 1 is the only route not to use ZSM-5. Perhaps research focus has been misdirected towards this zeolite.

Geographic Constraints again occupy a large score range, also the worst scored indicator overall. This may be indicative of future issues in finding appropriate locations, most routes requiring significant space and skilled engineers. A common constraint was the use of metals (complicating supply chain). Route 9 scored highly without a metal doped catalysts, a scalable, flexible one-pot process and the ubiquity of lignin feed. Intermediate scores were hindered by the requirement for specialist infrastructure or feed procurement such as algae ponds, syngas plants and carbon capture or point source CO_2.

Economic Feasibility was a highly uncertain semi-quantitative indicator and so expectedly those with institutional (Route 8) or commercial (Route 13) backing scored higher, rather than routes proving explicitly more/less profitable. Route 7 scored well due to the accompaniment of detailed economic calculations with literature. Optimistically, no routes were found to be economically infeasible at this stage and no particular component costs were found to be inhibitive. However, this is a reflection of low maturity and will likely change with further catalyst development. This will also strongly influence Energy Requirement, again currently highly uncertain. Significant across all routes (generally due to high temperatures and feed pre-treatment), Energy Requirement was also not a useful differentiator as any H_2 production requirements will likely exceed the remainder if produced via electrolysis. Many routes utilise hydrogen from other sources (biomass, methane etc.) but quantifying top-up requirements is not possible at low maturity. Routes with process simplicity and few feed pre-treatment steps (1 & 18) showed the lowest energy requirements.

4.1.4. Planet indicators

Route 15 showed strong Emissions Reduction Potential assuming biogas used would otherwise not be collected (i.e. without the economic incentive), hence offsetting significant methane emissions. Feedstock ubiquity proved beneficial, reducing the need for bulk transport via heavily polluting diesel powered ships. Most scores were intermediate, with low scores again representing uncertainty rather than definitively low reduction potential. A significant portion of emissions will arise from the end use of Benzene (e.g. combustion vs long term carbon storage in polymers) which is not route dependent. However, it is notable that compared to traditional benzene production, there is less qualitative variety in emission gasses and particulates (Ecoinvent, 2007).

General Environmental Performance showed little variation (highest incidence of '2' scores) with a similar level of fossil offset and the significant actor, reduction of finite metal resource, again difficult to quantify due to uncertainty in catalyst requirements. Route 11 was an exception to this trend, avoiding the use of metals and, by optimal use of algae, offsetting carbon emissions and preventing or taking advantage of eutrophication.

4.2. Application of weightings: scenario outcomes

When considering the scenarios, weightings were applied to each indicator based on pairwise comparisons between indicators. A consistency index was calculated to determine consistency across indicator importance within each of the 3Ps i.e. the similarity of AHP scoring. The acceptable limit is typically 10%. This level is exceeded by 'Planet': TRL contrasting with other indicators to result in consistency indexes of 21%, 25% and 25% (per case, 1–3). As the objective was not to be consistent within 3Ps, this is not considered a limitation although may still lead to unintended under or overrepresentation and suggests TRL may better fit within another, perhaps 'Profit' (Tables 3-5).

4.2.1. High performing routes

Across all three scenarios, Routes 1 and 9 continue to be ranked highest, Fig. 4.1. This strongly differentiates 1 and 9 from other routes as, regardless of stakeholder preference (across 'People', 'Profit' or 'Planet'), they retain desirability. In addition, arguably the best feature of each route (Carbon efficiency for 1, Geographical constraints for 9) is weighted low across scenarios, not impacting rank. 1 and 9 are also 2 of 3 routes with no zero values, implying generally that routes

Table 3
Weighted performance matrix for Scenario 1: Multi-National Corporation in Developed Country.

3Ps		Indicator		Route								
	Weighting		Weighting	1	2	7	8	9	11	13	15	18
People	0.333	Health & Safety	0.752	0.752	0.251	0.251	0.251	0.752	0.251	0.251	0.251	0.251
		Potential for Supply Chain Discriminatory Practices	0.248	0.165	0.165	0.083	0.000	0.331	0.331	0.000	0.083	0.083
Profit	0.333	Carbon Efficiency	0.116	0.155	0.039	0.077	0.039	0.039	0.039	0.039	0.077	0.000
		Geographical Constraints	0.039	0.013	0.013	0.000	0.000	0.052	0.026	0.013	0.000	0.013
		Economic Feasibility	0.566	0.377	0.377	0.566	0.754	0.189	0.189	0.754	0.377	0.566
		Energy Requirement	0.279	0.279	0.093	0.093	0.093	0.186	0.186	0.000	0.186	0.186
Planet	0.333	Emissions Reduction Potential	0.500	0.333	0.333	0.167	0.333	0.500	0.167	0.167	0.500	0.333
		Environmental Performance	0.500	0.333	0.333	0.333	0.167	0.167	0.500	0.167	0.333	0.333
		TRL	0.151	0.050	0.050	0.101	0.101	0.050	0.050	0.202	0.050	0.050
			Route Total	2.408	1.605	1.569	1.637	2.215	1.688	1.390	1.807	1.765
			Route Rank	1	7	8	6	2	5	9	3	4

A colour gradient is used as a visual aid to indicate relative scoring. Each colour represents 1/5 the range of achieved scores i.e. red represents the lowest scores a route could achieve for a given indicator, while dark green shows the top 5th.

perform well not due to single exceptional aspects, but for not neglecting any aspect of sustainability.

4.2.2. Low performing routes

Route 13 again performed the worst in both scenario 1 & 3 and ranked 8th in scenario 2, revealing that despite preference for high TRL (as in scenario 2), this is not enough to offset greater sustainability benefits in other areas or the increased uncertainty for this particular route. However, given the imminence of climate change, TRL should perhaps be given even greater weighting, although AHP does not allow for this, with the weighting extreme already occupied. Scores of zero were disproportionately influential on both advantageous and harmful indicators as remain zero regardless of weighting. The highest incidence of zero scores occurred in Geographical Constraints and Supply Chain Discrimination Potential and indeed, where weighted strongly in scenario 3, Routes 8 and 13 rank 8th and 9th. The ranking consistency for both top and bottom routes could be expected if intermediates were homogeneous, but this is not the case, further supporting the desirability of Routes 1 & 8 and the avoidance of 13.

4.3. Qualitative uncertainty analysis

Unexpectedly, containing only qualitative indicators, ‘People’ was less uncertain on average (49%) than ‘Profit’ (68%) or ‘Planet’ (81%) (see Fig. 4.2). Typically, quantitative indicators are more certain due to use of objective numerical values and structured methodology. This

Table 4
Weighted performance matrix for Scenario 2: Start-up in Developing World.

3Ps		Indicator		Route								
	Weighting		Weighting	1	2	7	8	9	11	13	15	18
People	0.311	Health & Safety	0.833	0.777	0.259	0.259	0.259	0.777	0.259	0.259	0.259	0.259
		Potential for Supply Chain Discriminatory Practices	0.167	0.104	0.104	0.052	0.000	0.207	0.207	0.000	0.052	0.052
Profit	0.493	Carbon Efficiency	0.148	0.292	0.073	0.146	0.073	0.073	0.073	0.073	0.146	0.000
		Geographical Constraints	0.105	0.052	0.052	0.000	0.000	0.206	0.103	0.052	0.000	0.052
		Economic Feasibility	0.491	0.485	0.485	0.727	0.969	0.242	0.242	0.969	0.485	0.727
		Energy Requirement	0.256	0.379	0.126	0.126	0.126	0.253	0.253	0.000	0.253	0.253
Planet	0.196	Emissions Reduction Potential	0.500	0.196	0.196	0.098	0.196	0.294	0.098	0.098	0.294	0.196
		Environmental Performance	0.500	0.196	0.196	0.196	0.098	0.098	0.294	0.098	0.196	0.196
		TRL	1.830	0.358	0.358	0.716	0.716	0.358	0.358	1.433	0.358	0.358
			Route Total	2.480	1.490	1.604	1.722	2.151	1.529	1.549	1.684	1.734
			Route Rank	1	9	6	4	2	8	7	5	3

A colour gradient is used as a visual aid to indicate relative scoring. Each colour represents 1/5 the range of achieved scores i.e. red represents the lowest scores a route could achieve for a given indicator, while dark green shows the top 5th.

Table 5
Weighted performance matrix for Scenario 3: Research Institution.

3Ps		Indicator		Route								
	Weighting		Weighting	1	2	7	8	9	11	13	15	18
People	0.196	Health & Safety	0.333	0.196	0.065	0.065	0.065	0.196	0.065	0.065	0.065	0.065
		Potential for Supply Chain Discriminatory Practices	0.667	0.261	0.261	0.131	0.000	0.522	0.522	0.000	0.131	0.131
Profit	0.311	Carbon Efficiency	0.604	0.751	0.188	0.376	0.188	0.188	0.188	0.188	0.376	0.000
		Geographical Constraints	0.085	0.027	0.027	0.000	0.000	0.106	0.053	0.027	0.000	0.027
		Economic Feasibility	0.173	0.107	0.107	0.161	0.215	0.054	0.054	0.215	0.107	0.161
		Energy Requirement	0.137	0.128	0.043	0.043	0.043	0.085	0.085	0.000	0.085	0.085
Planet	0.493	Emissions Reduction Potential	0.500	0.493	0.493	0.247	0.493	0.740	0.247	0.247	0.740	0.493
		Environmental Performance	0.500	0.493	0.493	0.493	0.247	0.247	0.740	0.247	0.493	0.493
		TRL	0.137	0.067	0.067	0.135	0.135	0.067	0.067	0.270	0.067	0.067
			Route Total	2.457	1.678	1.515	1.251	2.138	1.954	0.988	1.998	1.456
			Route Rank	1	5	6	8	2	4	9	3	7

A colour gradient is used as a visual aid to indicate relative scoring. Each colour represents 1/5 the range of achieved scores i.e. red represents the lowest scores a route could achieve for a given indicator, while dark green shows the top 5th.

likely results from use of quality sources but with lower applicability, without reflection in the assessment. For example, Supply Chain Discrimination Potential uses five consistent, high quality NGO or government sources, but that are also applicable to a country as a whole that may or may not constitute the eventual supply chain, neglecting specifics. Meanwhile, the requirement for specific values in quantitative indicators forced the use of less reliable sources and greater extrapolation. This is reflected in 'People' reliability scores equating or exceeding representativeness for every route, with highest certainty of all nine 3P/uncertainty indicator combinations.

While uncertainty was high for each 'P', 'Planet' was the most uncertain, achieving values of 100% uncertainty across Routes 2, 9 and 13. Found to be not representative and highly speculative due to a significant lack of data, perhaps 2, 9 & 13 'Planet' scores should be disregarded.

Route 9 is the most uncertain overall (averaging 86%), questioning its success in ranking. Low certainty may arise from non-use of metals; hence several evaluation methods may not be representative for this route. This can be verified by uncertainty in Route 11 (again without metal use), also with high uncertainty (69%). Here, the route effectively substitutes doped metal for excess HZSM-5 (20:1 catalyst to feed ratio) which, unrealistic for deployment, introduces much uncertainty around the final amount (and cost) of catalyst required.

That most preferred by industry (Route 13) is the amongst the least certain (72%), although this is arguably a reflection of information scarcity in open literature and is not representative of the technology. By contrast, that most favoured by a large research institution (Case 2 – Route 8) is relatively certain (53%).

4.4. Sensitivity analysis

The objective of the sensitivity analysis is to determine the relative influence of 3P weighting choices on final route rankings. The assessor belongs to a 'Western, Educated, Industrialised, Rich and Democratic' (WEIRD) culture and this, alongside other underlying bias, will have unavoidably influenced the scoring to some extent. In order to quantify, both relative to a reference case (Case 1) and to other 3P weighting alterations, a Pearson Correlation Coefficient (PCC) matrix was constructed, Fig. 4.3. The highest value of '1' indicates the change in weighting to have no impact on the final ranking (e.g. increasing 'People' wcrit by 5% has no impact on final rank vs reference case), while '0.98' indicates here that two ranks are swapped (e.g. decreasing 'People' wcrit by 25% vs reference case results in reversed ranks 5 and 6). A more extreme example, '0.48' for −50% vs +50% (i.e. 100% total) change in 'Profit' weighting shows every final rank to differ, the relative coefficient magnitude indicating to what extent.

A change of ±5% to any 3P weight made no change to rankings. ±25% Relative to Case 1 resulted in a lowest PCC of 0.9 (+25% 'Profit') with any given route at most 2 ranks away from reference. For all ±25% cases, no change to the most desirable routes (1 & 9) or single worst route.

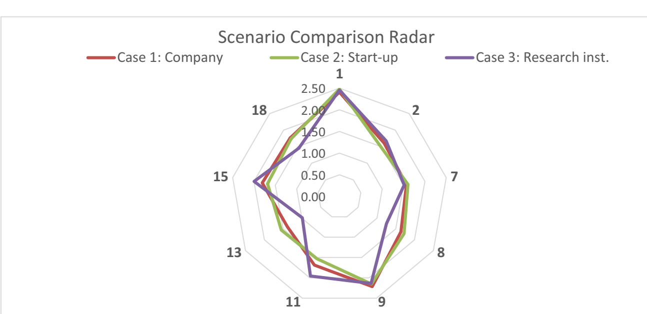

Fig. 4.1. Comparison of scenario by total scores for each route.

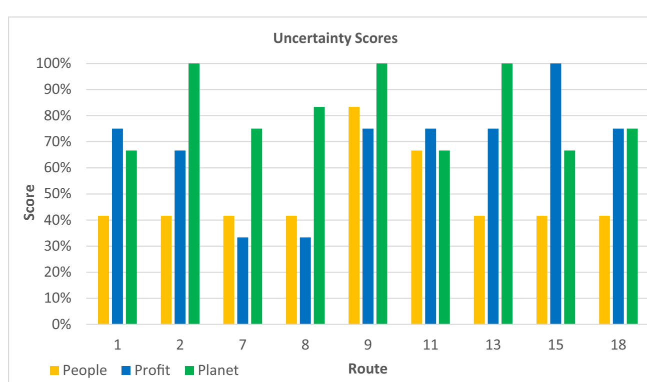

Fig. 4.2. Uncertainty scores per route and 3Ps.

			W People						w Profit						w Planet					
		Case 1	+ 5%	-5%	+25 %	-25%	+50 %	- 50%	+ 5%	-5%	+25 %	-25%	+50 %	-50%	+ 5%	-5%	+25 %	-25%	+50 %	-50%
	Case 1	1.00	1.00	1.00	0.97	0.98	0.90	0.87	1.00	1.00	0.90	0.97	0.75	0.88	1.00	1.00	0.98	0.95	0.98	0.90
w People	+ 5%		1.00	1.00	0.97	0.98	0.90	0.87	1.00	1.00	0.90	0.97	0.75	0.88	1.00	1.00	0.98	0.95	0.98	0.90
	-5%			1.00	0.97	0.98	0.90	0.87	1.00	1.00	0.90	0.97	0.75	0.88	1.00	1.00	0.98	0.95	0.98	0.90
	+25%				1.00	0.92	0.97	0.77	0.97	0.97	0.78	1.00	0.58	0.95	0.97	0.97	0.98	0.85	0.98	0.78
	-25%					1.00	0.82	0.92	0.98	0.98	0.93	0.92	0.82	0.80	0.98	0.98	0.95	0.97	0.95	0.93
	+50%						1.00	0.65	0.90	0.90	0.72	0.97	0.50	0.98	0.90	0.90	0.93	0.78	0.93	0.72
	-50%							1.00	0.87	0.87	0.93	0.77	0.83	0.62	0.87	0.87	0.83	0.90	0.83	0.85
w Profit	+ 5%								1.00	1.00	0.90	0.97	0.75	0.88	1.00	1.00	0.98	0.95	0.98	0.90
	-5%									1.00	0.90	0.97	0.75	0.88	1.00	1.00	0.98	0.95	0.98	0.90
	+25%										1.00	0.78	0.93	0.70	0.90	0.90	0.85	0.98	0.85	0.97
	-25%											1.00	0.58	0.95	0.97	0.97	0.98	0.85	0.98	0.78
	+50%												1.00	0.48	0.75	0.75	0.67	0.90	0.67	0.92
	-50%													1.00	0.88	0.88	0.92	0.77	0.92	0.70
w Planet	+ 5%														1.00	1.00	0.98	0.95	0.98	0.90
	-5%															1.00	0.98	0.95	0.98	0.90
	+25%																1.00	0.90	1.00	0.83
	-25%																	1.00	0.90	0.98
	+50%																		1.00	0.83
	-50%																			1.00

Fig. 4.3. Pearson correlation coefficient matrix.
A continuous colour gradient is used as a visual aid to indicate relative change i.e. red represents the highest impact of weighting change on final rankings, with dark green the lowest impact.

(13) occurred - arguably this is the most important outcome of the analysis. In addition, Route 15 (rank 3) was replaced in only two cases. This shows general high consistency in the results, with low overall impact from subjective decision making during the scoring process, and that the methodology used has significantly and meaningfully differentiated routes. +\-50% is less relevant, representing significantly different choices in weighting, although further emphasises consistency: the most extreme change from reference case rank was 0.87 (‘People’ -50%).

Although 3Ps are weighted equally in reference case (0.33), changing ‘Profit’ has had the largest overall impact to rankings (‘Profit’ vs ‘Profit’ averages 0.88 compared to 0.93 for ‘People’ and ‘Planet’, 0.95). This suggests routes closely aligned (i.e. overall score behind rank is not significantly different) are differentiated based on ‘Profit’ indicators, while those further from nearby rank are often based on ‘Planet’ indicators. Normalised 3P totals of unweighted scores are close (14, 14.75. 15.7), showing no particular route bias towards a given 3P, although this will be influenced by deliberate selection of scoring scale to differentiate routes and make use of extreme values (0, 4).

4.5. Limitations

Lack of data is the largest limitation to this study. This is highlighted by the high uncertainty of the ‘Planet’ category and is evident in wider uncertainty data. While acceptable at a screening stage, typically quantitative LCA indicators were necessarily only semi-quantitative here. Influential to all indicator scoring (including uncertainty), required catalyst quantities are largely unknown, and values used in low TRL studies are unrepresentative of industry. Relative amounts of hydrogen, feedstock and associated production methods are also difficult to speculate on at this stage, highly dependent on plant location, but with large impact on energy and cost. In particular, costs for materials derived from multiple sources (e.g. syngas from various biomass) or traded on global markets (e.g. benzene) are highly variable and figures used are subject to change. Although quantitative bias is weighted out, inclusion of more ‘Profit’ indicators does not provide the required balance to represent sustainability, but does highlight lack of social development for low maturity technologies. TRL could have been included in either ‘Profit’ or ‘Planet’ and, while justified, this study is unable to balance differing stakeholder viewpoints.

5. Conclusions

As a widely used chemical feedstock without alternative in polymer and high energy density liquid fuel production, the ability to produce benzene renewably from sustainable carbon feedstocks is a necessity for a future circular economy. Emerging technologies demonstrate that it is possible to produce renewable benzene from a variety of both catalysts and feedstock. However, all methods are of low maturity, developed in the last two decades. It is clear that benzene would not be produced in isolation (at least with current catalyst research veins), but rather as part of a wider biorefinery, producing a spectrum of hydrocarbons and/or aromatics. This is evidenced by the preference for the more valuable and widely used p-xylene and the low selectivity for any given aromatic even with the most successful catalysts. The pace of development and broad range of technologies researched highlight the difficulty of the situation: when should companies invest in deploying a promising technology if catalysts or routes of lower maturity with higher conversion and lower costs are on the horizon. Given the imminent issue of the climate crisis, and need for sustainable development, the incentive to wait is problematic.

For all three presented scenarios, Route 1 (closely followed by 9) ranked highest with strong performance across the 3Ps, 'People', 'Profit' and 'Planet'. Route 1 coupled the use of an Fe/Fe_3O_4 nanoparticle catalyst with CO_2/H_2 feed to produce benzene, while Route 9 pyrolyses a lignin feed in the presence of HZSM-5 to achieve subsequent aromatisation of the gases. Success was attributed largely to the process and feedstock simplicity of each route having a wide, positive influence on multiple indicator scoring. Sensitivity analysis confirmed a lack of assessor bias in the weightings and ultimate ranking, showing significant variation only in $\pm50\%$ weight changes; further grounding 1 & 9 as the best routes regardless of scenario. Both are low TRL, whilst the least successful (13) occupies the highest TRL, contrasting with real industrial decisions. Arguably, this outcome is due to the nature of available literature and is not representative of the technology itself. Much industrial interest focusses on the use of pyrolysis as a currently viable production route for a range of hydrocarbons. For example, Anellotech (2019) was considered but, as above, lack of available data prevented further analysis. Often ranking 3rd, Route 15 (Mo/ZSM-5 catalysed dehydroaromatisation of methane) also showed promise largely due to methane emission offset and, alongside 1 and 9, is worthy of more detailed analysis in further work.

Given the advantages and disadvantages of each route in differing areas, it seems likely that any industrialised route would combine aspects from a variety of those reviewed. Aspects could be easily interchanged where common intermediates such as syngas or methanol are used. For example, the iron oxide nanoparticle catalyst from Route 1 is the most successful but uses a feed of CO_2 and H_2. Using hydrogen in this way may prove energy intensive, but the first step of the reaction mechanism is conversion to syngas and so alternative use of a biomass-derived syngas feed may prove more feasible. Although currently underperforming in the context of sustainability as the youngest research, Route 18 has made fast progress in recent years. Use of a CO_2 feedstock in a one- pot process may become increasingly desirable if carbon taxes are introduced, potentially increasing competitiveness against Route 1.

In summary, the primary goal of this study was to identify and compare feedstocks and routes to the production of renewable benzene and, assuming the deploying entity values sustainability above cost and convenience, this has been successful. However, a comparison to traditional production from crude oil could also be conducted, potentially revealing or quantifying the additional value and costs derived from renewable production. Due to the emerging nature of all routes, assessment rankings are likely to change with developmental research and subsequent scale-up. New routes will emerge possibly combining attributes rather than utilising any single route assessed here. Therefore, the model developed with this work allows new routes to be added, process data to be updated and priorities altered; thus enabling practitioners to continue to assess new routes to renewable benzene as they develop. Ultimately, the sustainable deployment decision will depend highly on geographic location, local availability of a given feedstock and compatibility with an effective catalyst.

CRediT authorship contribution statement

David Miller carried out the detailed analysis for the work and contributed to the writing of the manuscript. Katy Armstrong was a co-supervisor and contributed to the writing of the manuscript. Peter Styring was Principal Investigator on the project and co-supervisor, and helped in the editing of the manuscript.

Declaration of competing interest

There are no conflicts of interest.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.spc.2022.04.019.

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