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A defossilised EU petrochemical production system: Consequences for the meta-cluster in the Antwerp-Rotterdam-Rhine-Ruhr Area

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ABSTRACT

Today's petrochemical industry relies on fossil hydrocarbons, not only for energy purposes but also as feedstock. This use of fossil materials is being challenged by the European Union's target to achieve climate neutrality by 2050. The most affected region in Europe is the cross-border region between Antwerp, Rotterdam and the Rhine-Ruhr area in western Germany, an interconnected petrochemical meta-cluster. Although several defossilisation scenarios for petrochemicals have been developed both at the EU level and for single countries, the effect that an EU-wide transition from fossil to non-fossil feedstock would have on technology routes, feedstock alternatives and final product shares, as well as the resulting locational and geographical consequences are not yet understood. To fill this gap, the paper presents a scenario where the European petrochemical industry transitions away from fossil by 2050 and analyses how the energy supply and the defossilisation of carbon supply will change this industry. With this scenario as a backdrop, a zoom-in shows how the Antwerp-Rotterdam-Rhine-Ruhr Area might evolve technically and spatially. To this end, a techno-economic bottom-up model is employed that derives costoptimal pathways towards defossilised petrochemical production networks. The analysis shows that a scenario for petrochemicals that achieves full non-fossil feedstock use in the EU by 2050 is very likely to be associated with a significant change not only in the feedstock base but also in the production technologies. The meta-cluster will face major challenges as its current strength in specialty polymers might suffer from cost increases for aromatics and the high energy intensity of the respective polymerisation steps. This requires specific strategies in regard to feedstock and energy supply as well as infrastructure.

1. Introduction

The EU has the ambition to become the first climate neutral continent by 2050 as part of fulfilling the Paris Agreement [1]. For the petrochemical industry, this is an unprecedented challenge as the industry relies heavily on fossil hydrocarbons, not only for energy purposes but also as the main feedstock embodied in their products. Achieving carbon neutrality will thus require transformative changes in both production processes and material inputs.

While strategies involving Carbon Capture and Storage (CCS) are often highlighted as a key enabler for climate neutrality, relying solely on CCS without addressing the fossil-based nature of the feedstock may fall short in achieving the long-term goals of climate neutrality. Defossilising the feedstock, when combined with CCS, offers an additional and essential pathway to reducing greenhouse gas emissions. This dual approach not only amplifies the potential for emission reductions but also creates a safeguard against the uncertainties surrounding the scalability, cost, and timely deployment of CCS technologies.

Moreover, defossilised feedstocks contribute directly to the structural reduction of carbon inputs into the system, paving the way for the generation of negative emissions—an essential requirement to offset residual emissions and adhere to the Paris Agreement's more ambitious climate targets. As we approach the emission reduction deadlines set by the EU, the visions and demands to defossilise petrochemicals are no longer nascent; they are becoming increasingly urgent. This urgency underscores the need to integrate feedstock defossilisation into the broader decarbonization strategy of the petrochemical sector, ensuring a resilient and comprehensive transition to climate neutrality.

Apart from climate challenges, the petrochemical sector also faces several other environmental issues such as poor recycling rates and

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plastic pollution. There is thus a growing public pressure to increase circularity and reduce untreated waste streams, particularly plastics, as exemplified by the recently adopted policies on circularity [2] and policy for reducing single-use plastics [3].

Petrochemical production plants are typically concentrated in clusters due to energy- and feedstock integration opportunities and access to infrastructures such as harbours, pipelines etc. [4] The European chemical industry consists of several geographical clusters but the ARRRA (Antwerp-Rotterdam-Rhine-Ruhr Area) cluster is the largest and most integrated petrochemical cluster in Europe. Around 50 % of European platform chemicals are produced here. Phasing out of fossil fuels and feedstock will not only be an immense challenge for the economy and the energy system but will have manifold structural consequences for this highly complex and meshed petrochemical production- and use-system.

Several studies have analysed possible technical pathways away from fossil energy and feedstock in the petrochemical industry with early works focussing on hydrogen with captured CO₂ [5–7], or using biomass as feedstock for replacing fossil material [8] or a combination of hydrogen and biomass [9]. Later contributions have included increased circularity and the utilization of waste streams as carbon feedstock, or any combination of all the above options available in optimization models including also demand management [10–12].

With a shift away from fossil energy and feedstock, the benefits of integration and availability of cheap fossil resources will change radically and thus also the spatial configuration of clusters. Non-fossil materials that can replace fossil feedstock for petrochemicals are organic waste streams, biomass and renewable hydrogen combined with captured CO_2 . These feedstocks will have different integration benefits compared to oil and gas and they will be accessible at different locations compared to today's fossil feedstock naphtha, ethane and reformate that are derived from oil and gas respectively.

While the transition to new non-fossil feedstocks may be straightforward for mono-structured and vertically integrated chemical parks, the issue will be particularly complex for the highly horizontally integrated European meta-cluster ARRRA. Here, too, the transition to new non-fossil feedstocks, whose yield structures are not comparable to today's crude oil-based feedstocks, can have a severe impact on the horizontal organisation of the cluster.

The effects that an EU-wide transition from fossil to non-fossil feedstock would have on technology routes, feedstock alternatives and shares of final products, as well as the resulting locational and geographical consequences are, however, not yet understood.

The aim of this paper is to fill this gap and to develop a scenario where the $EU27+3^{1}$ petrochemical industry transitions away from fossil to non-fossil fuels and feedstock by 2050 and analyse how the energy supply and the defossilisation of carbon supply will change this industry and what policy levers might be needed to incentivise the transition. With this scenario as a backdrop, we then zoom in on the ARRRA-cluster and analyse how this highly integrated and geographically concentrated meta-cluster could technically and spatially develop.

To this end, we employ a techno-economic bottom-up model that derives cost-optimal pathways towards a defossilised petrochemical industry. In order to incentivise gradual defossilisation, we assume a rising tax on the use of fossil carbon as a technical model parameter. In reality, such a tax (or quotas on non-fossil feedstock) could be a complement to the pricing of end-of-life emissions through the EU ETS. With the availability of CCS as a technology option to address end-of-life emissions, the EU ETS alone is not sufficient to incentivise defossilisation.

The model optimises investments in key production assets and plant operations, taking into account, for example, energy and feedstock integration opportunities and costs for new investments, transport costs and sunk costs associated with existing assets.

The paper is structured as follows: First we provide a systematic overview of the highly meshed European petrochemical production system, with a view on its main energy intensive production steps, its geographical distribution and its infrastructural links. In this section we also elaborate on what makes the ARRRA a unique meta-cluster. Second, we present our methodology, with the assumptions presented in the third section. The fourth section shows the results of a defossilisation scenario for the European petrochemical industry as a whole and based on this scenario section five presents a deep dive analysing the resulting reconfiguration of the ARRRA cluster and its robustness. In our conclusion, we provide a structured overview of how climate neutrality will reconfigure the European petrochemical industry and the ARRRA cluster and what challenges as well as strategy and policy options emerge.

2. The European petrochemical production system

The European Union produces around 50 Mt of fossil based primary polymers per year, 6 Mt recycled plastics and 1.3 Mt of bioplastics [13]. In our analysis, we cover all steps of the production chain from the feedstock to the primary polymers. Ammonia has only been included for its use in the production of polymers (see Fig. 1) and not for its use in the fertiliser industry. To categorize the different inputs, intermediates and final products in the system we use the following terms, which can also be found in Fig. 1:

- 1. *Feedstock* is typically produced outside the chemical production system such as crude oil and its components (like naphtha and LPG), natural gas, wood or natural salt as well as air for nitrogen, oxygen and CO₂.
- 2. In the first stage of the petrochemical production the feedstock is converted into A) high-value chemicals (*HVC*) such as olefins (ethylene and propylene butadiene) and aromatics (benzene, toluene and xylenes often abbreviated as BTX) and B) *platform chemicals* such as methanol, ammonia, chlorine, and hydrogen.
- 3. HVCs and platform chemicals are converted into *polymers*, in one step as in the case of polyethylene (PE) and polypropylene (PP) or in several steps via *intermediates* such as monomers and their precursors.
- 4. Polymers are the end products of the (petro-) chemical industry. They are typically treated physically by the downstream "plastic converters". In regard to polymers, we differentiate between four groups:
 - a. Commodity plastics
 - b. Engineering plastics
 - c. Polyurethanes (PUR)
 - d. Rubbers

Today's petrochemical production pathways in Europe are sketched in Fig. 1. The Sankey diagram illustrates that the hydrocarbon feedstock in Europe can almost exclusively be traced back to by-products from crude oil refining.

The 40 million tons of HVC that are produced in the EU-27 consist of six hydrocarbons which are then further converted into polymers. For the production of polymers other than PE and PP, further production steps with intermediates are required. Some of these intermediates need other organic or inorganic chemical building blocks coming from 'platform chemicals' such as chlorine, ammonia, methanol and hydrogen.

The map in Fig. 2 shows that the ARRRA meta-cluster is the heart of the petrochemical production system in Europe. It has several relevant characteristics that differentiate it from other European clusters and that may accelerate or impede its transition to defossilisation: It consists of a number of refineries and petrochemical production sites, often co-located. In addition, the ARRRA has several chemical production sites

¹ EU27+3 denotes EU 27, UK, Norway and Switzerland.



Fig. 1. Sankey-diagram for the polymer production system in the EU27+3 region (sizes reflect mass-flows of the current petrochemical system, modelling results). HVC = olefins (ethylene (C2H4) and propylene (C3H6)), butadiene (C4H6) and aromatics or BTX (benzene (C6H6), toluene (C7H8) and xylenes (C8H10)); platform chemicals = ammonia, molecular chlorine, hydroxyl groups (methanol), molecular hydrogen; for explanations to polymers see Fig. 3; LLD-PE included in LD-PE. Source: own figure.



Fig. 2. Map of petrochemical production capacities in Europe (EU27+3, state of capacity data: 2020). Source: own figure.

that can be characterised as "chemical parks", which are themselves clusters integrating many local energy and material flows. These clusters are linked by an extensive (pipeline) infrastructure that allows a significant volume of material and energy exchange between the sites. The ARRRA cluster is thus a meta-cluster consisting of several strongly interconnected local clusters. This structure has adapted over time with regard to the available crude oil by-product yields from the refineries in ARRRA [4] and today represents a strong lock-in to the established polymer production portfolio and the demand structure for plastics that has co-evolved with it.

Most other chemical clusters have limited production portfolios and are focused on commodity plastics with low conversion depth. The ARRRA cluster, however, benefits from a broad portfolio with multiple synergies and flexibility within the cluster, as well as a range of additional conversion steps that can respond to changing upstream and downstream market developments (see Table 1). In particular, its position in engineering plastics and polyurethane (PUR) foams is very strong: The ARRRA meta-cluster dominates the European supply for PC, PA, ABS and PMMA as well the main ingredients to produce PUR foams (polyols, MDI & TDI). These polymer types are particularly relevant for the manufacturing of cars and machinery like electric and electronic devices [13] and are thus crucial parts of key industrial value chains in Northwestern Europe. Apart from Geleen, all major clusters within the ARRRA meta cluster produce those polymers. This level of horizontal integration and conversion depth can only be found in very few clusters outside the ARRRA such as Middle Germany and Tarragona.

The European plastics production system is largely, but not entirely, self-reliant as there are systematic net trade flows for some products, but these are relatively small compared to total production and demand. The European polymer production system can thus be seen as a stable system and is therefore treated with limited connections to the world market in our model. Future polymer trade flows between Europe and other world regions are thus not explicitly modelled. All scenarios explored assume trade restrictions for fossil-derived by-products at all stages of the value chains. Modelling future trade flows between Europe and the rest of the world would therefore require explicit assumptions about the future trade regime for petrochemicals and about green polymer production in the rest of the world, which is beyond the scope of this paper.

3. Methodology

3.1. Model description

We employ a linear cost-optimization model that optimizes simultaneously investments and use for 50 different types of petrochemical production assets, including novel non-fossil production routes as well as decarbonized energy supply. The model scope is the European production system. The world market is not covered with the exemption of feedstock, which can be imported. The model optimises a) the technological and spatial distribution of new investments and b) the utilization rates of all chemical production assets taking into account existing assets, reinvestment needs and transport infrastructures. In the core scenario (see scenario analysis concept in the supporting information, SI), the optimisation procedure uses perfect foresight over a period of 20 years, which represents a usual time horizon in the planning of strategic investments in companies. The cost assumptions used for future alternative feedstocks and technologies are based on literature reviews and expert knowledge (see SI). The modelling is conducted under the condition of a full defossilisation of the European chemical production system by 2050 where the model analyses the resulting changes in competitiveness between European regions and relative positioning of sub-clusters. These lead to different patterns of reinvestment and utilisation of assets. The analysis includes the EU, Norway, UK and Switzerland (EU27+3). Changes in competitiveness relative to overseas production are not taken into account.

The simulation builds upon three major input data sets: (1) the

European demand for primary polymers over time, (2) the availability of waste for chemical recycling over time and (3) today's existing assets in the European petrochemical production stock.

Demand for polymers and waste generation are derived by a dedicated plastics use model. We use a material flow analysis tool to precalculate plastic use in Europe. The results of the module are given below and detail on the methodology is presented in the SI. These results are used as an input to the optimisation model presented here. The background data on the existing production stock is taken from a database developed in several projects at the Wuppertal Institute, which includes all major sites with specific facility level description, free standing facilities, plus all relevant infrastructures such as pipelines and harbours. The database accounts for existing production stocks for feedstocks (crude oil refining), platform chemicals, high-value chemicals, intermediate products as well as polymers. All processes listed in the database are described by their location, annual production capacity, their specific material input and final energy demands according to literature values. For HVC producing stock (like steam crackers and FCC plants) individual plant age is also accounted for. The database contains around 1'000 individual plants of the chemical industry in the EU27+3. For the analysis here we focus on 50 petrochemical plant types, but we aggregated some of individual sites to "clusters" to reduce the complexity of the model. As a result, we consider 155 European production clusters that are represented by 664 processing units of 50 different process types in 2020.

Existing as well as future technologies are defined with the above described level of detail in the model in order to optimise a relevant transition path. The optimisation procedure of the model will choose for capacity investments, that are either replacement of retired processes or necessary due to growing needs of certain processes, between technologies with fossil feedstock and technologies with alternative feedstock. The model also simultaneously optimises the use of the plants towards a minimum cost solution on the level of the overall system costs using several boundaries presented below in Section 4 and described in more detail in the SI.

Fig. 3 presents the actual set of non-fossil technologies available to the model for meeting a strict requirement for a fossil-free polymer production (>2045) with waste, biomass and CO₂ as non-fossil carbon feedstock and water electrolysis as the core hydrogen production process. The major production processes for producing fossil free high-value chemicals (HVCs), are (1) steam cracking of waste based pyrolysis oils or synthetic Fischer-Tropsch-oils and (2) the methanol-based MtO/MtA processes, with the methanol coming either from waste or from the synthesis of CO₂ and hydrogen. Biomass can feed into both of these but can also be converted directly into biopolymers via bio-intermediates, see (3) in Fig. 3. Biomass can thus deliver either new kinds of polymers potentially substituting established polymers (e.g. PLA as a substitute for PS), deliver platform chemicals (like ethylene produced from ethanol) or even intermediates (e.g. adipic acid from biomass instead of producing it from benzene via cyclohexane).

For waste, we consider mechanical recycling in the pre-calculation of the demand for new polymers and available waste streams. In this material flow analysis tool, mechanical recycling is prioritized and the respective waste flows are not made available for other routes. The recyclate output is subtracted from the respective polymer demands resulting in the demand for new polymers. The remaining waste streams can be processed within the optimisation by the two chemical recycling routes that use plastic waste as a feedstock. Plastic waste pyrolysis produces pyrolysis oil that can be converted to HVC in a (slightly modified) steam cracker. Pyrolysis requires well-sorted waste as an input consisting mainly of polyolefins, i.e. PE and PP. [14,15] It was assumed that polyolefins from packaging can be mobilized for chemical recycling in the future. The gasification route on the other hand is more flexible and can handle also mixed (and partly contaminated) waste as an input. [16] It produces a syngas that can be converted to methanol and then further processed via either the MTO process to olefins or to

Table 1

Top-20 polymer production clusters in Europe and ARRRA share in total European polymer production capacities. Source: own analysis based on the Wuppertal Institute's database on production plants in Europe.

Cluster Region Commod			mmodity plastics						Engineering plastics					PUR foam ingredients			Rub-bers		
		HD-PE	LD-PE	LLD-PE	PP	PVC	PS	E-PS	PET	PC	PA 6/6.6	ABS	PMMA	SAN	polyols	MDI	TDI	PBR	SBR
Flanders	ARRRA	x	х		x	x	х	x	x	x	x	x			x	x			
Emscher-Lippe		x	х	x	х	х				х	x					х		х	
Rheinland		x	х	x	х	х						х			x		х	х	
Rotterdam					х	х			х		x		х		x	х		х	
Ludwigshafen							х	x			х	х	x	х			x**		
Geleen		x	х	x	х	х													
Terneuzen			х	x								х		х	x				
Middle Germany	Germany*		х	x	х	х	х	х	х		х							х	х
Rhône delta	France	x	х		х	х									x				
Le Havre		x	х		х		х												
Dunkirk						х	х	х				х							
Tarragona	Iberian Peninsula	x	х	x	х	х						х		х	x	х			
Puertollano		x	х		х										x				
Porvoo	Northern Europe	x	х	x	х		х	х											
Stenungsund		x	х	x		х													
North-Eastern Italy	Italy		х		х		х	х				х		х					
Szazhalombatta	Central Europe	x	x		х			х							x				х
Plock		x			х	х			х								х		
Kralupy							х	х										x	х
Grangemouth	UK	x		x	х														х
ARRRA share in total EU27+3 capacity [%]		43	44	34	38	33	44	32	21	67	50	69	90	37	65	49	40	38	-
Share of Northwestern	a Europe in EU27+3 [%]	43	46	40	46	48	50	37	31	79	72	69	90	37	70	75	40	66	27

*) Germany without the sites that are part of the ARRRA region;. ***) closed in 2023.

HD-PE = high-densitiy polyethylene; LD-PE = low-densitiy polyethylene; LLD-PE = linear low-densitiy polyethylene; PP = polypropylene; PVC = polyvinylchloride; PS = polystyrene; E-PS = expanded polystyrene; PET = polyethylene terephthalate; PC = polycarbonates; PA 6/6.6 = polyamide; ABS = acrylnitril-butadien styrene; PMMA = polymethylmethacrylate; SAN = styrene acrylonitrile resin; MDI = methylene diphenyl diisocyanate; TDI = toluene diisocyanate; PBR = polybutadiene rubber; SBR = styrene-butadiene rubber.

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The non-fossil petrochemical system shown here differs massively from the fossil system shown in Fig. 1, both in terms of its feedstocks (step 1) and the role of platform chemicals (step 2). Waste, biomass and CO₂ become the core carbon feedstock instead of fossil refinery by-products, and water electrolysis becomes the core hydrogen production process, with no changes to the inorganic feedstocks NaCl and nitrogen.

The HVCs (now step 3) are either still produced by steam cracking of then non-fossil Fischer-Tropsch based synthetic naphtha or (with the notable exception of butadiene) via MtO or MtA processes from the platform chemical methanol. Methanol, which is already used in small quantities as a platform chemical for PMMA, will thus potentially become a major feedstock for most non-fossil plastics. The gasification of steam cracking by-products (methane and gasoil) could deliver syngas for additional methanol production ("SC by-product methanol") and thus combine the two routes.

The final step from HVCs to polymers will remain largely unchanged technically, but bio-intermediates will also become alternatives to HVCs for the production of certain bio-polymers via specific routes.

aromatics via the MTA process.

Which of the alternative non-fossil HVC production routes is economically more attractive depends on the respective feedstock costs and on the relative values of the different products. An overview of how they perform in the context of the scenario developed here is presented in Section 5.1 below.

3.2. Definition of the core scenario

In the core scenario, the use of fossil carbon as energy and feedstock is subject to increasing costs and no fossil inputs are allowed after 2045. The displacement of fossil carbon leads to significant changes in the relative costs of various polymers (see Fig. 7) due to the different yield structures of the non-fossil routes compared to the existing fossil routes, and consequently to massive changes in the technical and locational structure of the industry. However, it can also be expected that these changes will lead to changes in the polymer demand structure of the plastics producing industries, which is not captured in our model. To anticipate some of the potential demand responses we variated the demand structure that is used as an input to the optimization model. The core scenario was calculated with regional energy price deviations within Europe and its robustness was further tested with sensitivity analysis including marginal cost analysis and stress tests (see Section 3 in the SI).

4. Scenario assumptions

To develop the defossilisation scenario for the European petrochemical industry, a number of broad assumptions have been made that describe the framework in which the industry will develop over the three decades to 2050, and a number of drivers that simulate the policies that will lead to defossilisation. As an overall context, we assume that the world will evolve in a general direction determined by the maintenance of world markets and trade, industrial growth and global cooperation plus strong multilateral climate policies, following roughly the philosophy of the IPCC's SSP1 storyline [17].

Within this context we identify four sets of framework developments over time that will largely determine the future configuration of the petrochemical industry. These are the assumed trends in feedstock demand and supply, the evolution of (green) energy availability and costs, infrastructure development and refinery capacity.

First, the central framework of the scenario is the expected physical trends in material demand and supply; e.g. plastics demand by sector and product, waste availability and cost (which is dependent on product demand in previous periods), biomass availability and cost, and trade balance of products and non-fossil carbon (e.g. as green methanol). For simplicity, we assume that the polymer demand structure of each plastic-consuming sector remains stable over time. The only exception to the business-as-usual is the demand for polymers in packaging. Here we assume saturation in 2030 due to higher material efficiency, less packaging and substitution of plastics by other materials. The resulting mass



Fig. 4. European plastic demand by industry and waste amounts used as an input for the production chain optimisation.

The figure shows that polymer production is expected to grow until 2050, with packaging losing share. Due to the constant increase in production, the amount of waste as a potential carbon supply will always be lower than the production volume, a fact that is aggravated by the constant high proportion of plastic losses. However, the recovered plastic, which today is mainly incinerated or exported, will increasingly be used for chemical recycling. Source: own figure.

balance of the overall plastics demand and waste availability over the next four decades is given in Fig. 4. It shows that, despite more efficient use of plastics, their overall demand is expected to grow, as it has in the past. We emphasise that the baseline polymer demand structure based on a stable polymer demand structure for each major use case (e.g. in packaging) is not a likely development. With the different changes in marginal costs of production due to defossilisation, as presented in the results section below, substitution effects between polymers can be expected. The first sector in which such substitution is likely to occur is packaging, where benzene derivatives such as polystyrene (PS) and polyamide (PA) which bear very high marginal cost can in most cases be easily replaced by polypropylene (PP) or low-density polyethylene (LDPE). An associated "second round effect" of such a substitution is an increasing proportion of polyolefin waste, which can later be used in the steam cracker route, providing additional (very valuable) butadiene yields. The presented case, with structural adjustments in the demand of packaging polymers, was the input to the subsequent optimisation model and therefore represents our "polymer demand and waste scenario" and the basis for the "core scenario" (see scenario analysis concept in the SI).

On the waste side, the contribution of mechanical recycling to meeting part of the future demand for polymers increases but remains limited due to limitations in varietal purity of plastic waste and recyclate input shares. The share of chemical recycling is growing rapidly. By 2040, about 85 % of the available plastic waste will be sent for chemical recycling and the rest for mechanical recycling. Fig. 4 also shows that the losses in the whole system are quite high, with 37 % of the "expected" waste amount from the modelling of the plastic use phases for 2020 not appearing in the waste statistics.² We assume that the proportion of unexplained losses remains stable over time.

The *second* key driver is the availability and cost of (green) feedstock and energy for the petrochemical industry in different parts of Europe, including the cost of emitting or using fossil carbon. Fig. 5 shows assumed world market prices for the three main fossil feedstocks (naphtha, ethane and propane), as well as expected world market prices of non-fossil feedstocks (synthetic naphtha and methanol) normalised to their energy content. The costs of the fossils will increase by about 10 % per decade. However, if their use were subject to a carbon tax, as assumed in the scenario, their prices would roughly triple by 2050. In this case non-fossil feedstocks may become competitive by 2040.

With a CO₂ tax development from $\notin 100/t$ in 2030, $\notin 250/t$ in 2040 to $\notin 300/t$ in 2050 on fossil feedstock, green methanol will be the cheapest feedstock in 2050, and already in 2040 it will be almost at parity with fossil ethane. The assumption about the price of green CO₂ and hydrogen based methanol is similar to other studies, e.g. Bazzanella and Ausfelder [18], who assume higher costs in 2040, but similar production cost in 2050. This is due to the relatively low investment costs and the good overall energy efficiency of converting electricity via hydrogen (and CO₂) to methanol. Green naphtha, on the other hand, could not compete with fossil naphtha in 2040. Only by 2050 would it be cheaper than fossil naphtha, but remain about 50 % more expensive than green methanol. However, this comparison does not take into account the different revenue structures in the processing of methanol and naphtha. An economic assessment based on the 2050 price assumptions is presented in Section 5.1 below.

Unlike feedstock, the energy price development is region specific. The respective assumptions are presented in the SI. We assumed a phaseout of natural gas use for heat supply until 2040 in Europe. Heat can thus be supplied by burning of by-products and electrification. For the ARRRA region we assumed a stable price for electricity in the BeNeLux region and for Germany. For other regions in Europe, we assumed also stable electricity prices except for Spain and Portugal, where renewable potentials are excellent and have not been exploited so far. In sum, this assumed development in the core scenario represents already a kind of general "investment stress test" to the ARRRA (see a discussion in Section 5.2) as the region loses its competitive edge over other regions like France, Sweden, Spain and Portugal.

The *third* framework is the geographical development and redeployment of infrastructure for the supply of raw materials and intermediates. The ARRRA region, in particular, has an extensive and diverse network of pipelines for feedstock and intermediates that can be

² See also Material Economics [21] who try to analyse the difference.



Fig. 5. World market price scenario for feedstock. Source: Own calculations.

repurposed in the context of structural changes in petrochemical production.

The fourth framework is the expected change in refinery capacity and the future location of both fossil and novel non-fossil refineries, which is assumed to be driven more by the transformation of the transport system than by the petrochemical industry. A climate-neutral Europe implies that the transport sector will phase out the use of fossil fuels, which will lead to the gradual closure of refineries. If the refineries are closed, the corresponding naphtha, propylene and benzene supply ceases and the associated petrochemical clusters lose their local supply. In this case they will source waste or alternative feedstock directly from the world market (at a higher price) if located on the coast or from a port via a naphtha pipeline or by rail. The phase-out of fossil crude oil refining in Europe is assumed to start in the late 2020s and to be completed by 2045. In parallel, we expect Europe to build new green hydrocarbon production capacity to supply non-fossil fuels, e.g. for aviation. Although these synthetic fuels could be produced more cost-effectively outside Europe, we assume that energy security reasons will favour some production within the EU (see SI). While the above developments will strongly guide the development of the petrochemical industry, we believe that the defossilisation of petrochemical production will be centrally driven by policies that put a price on both emitted carbon from combustion and also on carbon embodied in products. Policy is here modelled as a fossil carbon tax on both chemical feedstock and emissions. We also assume a complete ban on the use of fossil carbon in the EU by 2046. The impact of such a fossil carbon tax on feedstock prices is shown in Fig. 5.

5. Scenario results and discussion

5.1. Scenario of a future EU petrochemical production system

To reach carbon neutrality, the European petrochemical industry will significantly change over the coming decades. Table 2 shows the change in feedstock composition and the GHG equivalents from the embodied carbon.

In the decade after 2025 embodied GHG equivalents are already 1/3 lower compared to the current decade and are further reduced to 80 % lower after 2035. After 2045, the aim of non-fossil petrochemicals is assumed to be achieved. While almost all HVC production in 2020 was based on three main fossil routes, steam cracking, FCC and catalytic reforming, this will have changed completely by 2050 (see Fig. 6). Starting already before 2030 the MtO route will provide an increasing share of HVCs, with the carbon stemming from pyrolysis of waste. By 2040 the non-fossil MtO route provides over 50 % of all HVCs. After

Table 2

Technical key performance indicators of the core scenario. Source: Own calculations.

	[unit]	2016-2025	2026-2035	2036-2045	2046-2055
Total new polymer production Shares of carbon	Mt/a	42.7	43.9	45.3	46.0
feedstock					
fossil	%	100 %	82 %	20 %	0 %
waste	%	0 %	14 %	44 %	31 %
biomass	%	0 %	2 %	7 %	11 %
synthetic	%	0 %	2 %	29 %	58 %
green					
Carbon conversion to products	%	74 %	79 %	77 %	67 %
Feedstock	Mt	169	117	31	-
related	CO _{2eq} /				
GHG	a				
emission					
equivalents					

2040, new investments mainly go into non-fossil MtA which produces almost a quarter of HVCs by 2050, however with a considerable excess of para-xylene.³ In addition, after 2030 the carbon input for steam cracking is increasingly converted from fossil to non-fossil waste-based feeds: As can also be seen in Table 2, from 2026 to 2035 about 90 % of all feedstock is still fossil. However, in the following decade fossil carbon makes up for <50 %. In the last decade, after 2045 no fossil carbon is processed anymore. Over the period, HVC production initially declines slightly but returns to the 2020 level of around 43 Mt/a in 2050. Compared to the plastics demand, which is expected to grow steadily from 50 to 58 Mt/a between 2020 and 2050 (see Fig. 4), the decline in HVC production until 2040 can be explained by the increased use of mechanical recycling and the diminishing "exports" of toluene and

³ The assumed MtA process specification yields para-xylene as the main product and only small amounts of benzene and toluene. However, benzene supply is the main bottleneck in the system in 2050. Recent literature on the simulation of a new MtA process design [22] suggests that it may be possible to significantly increase the overall BTX yield, and benzene yield in particular at the expense of para-xylene, by using a more capital intensive two-stage fluidised bed reactor, which would likely improve the economics and system compatibility of the process.



Fig. 6. Production of HVCs in the EU by route and **feedstock**, 2020 to 2050. Source: own figure.

xylenes to the petrol market or to the chemical industry outside Europe. The increase after 2040 is then due to excess production of para-xylene.

Fig. 7 gives some reasons for the pattern of change in petrochemical production routes. MtO as well as steam-cracking based on pyrolysis oils from waste have by far the lowest production costs of all non-fossil routes of 700 and 850 \notin per ton of HVC produced and a significantly higher expected revenue.⁴ This means the waste based routes will be the first to replace fossil based production after 2035 when the tax on fossil carbon is high enough to make them competitive.

MtO fed with imported DAC⁵-based methanol has production costs of almost 1100 \notin per ton, but is still significantly cheaper than MtA based on imported DAC-based methanol or steam cracking based on imported DAC-based naphtha, which both have production cost of roughly 1800 \notin per ton of HVC. However, after 2040 most of the investments are directed into the MtA route due to its capability to produce benzene, toluene and para-xylene, which are rare from the waste-based routes, but still needed for certain products.

Table 3 shows the necessary investment and cost patterns of the transition. The investments into non-fossil routes slowly start after 2025 but increase massively between 2036 and 2045. In the latter decade a huge production capacity is erected for waste pyrolysis and gasification as well as new MtO capacities (see Fig. 6). After 2045 investment into new HVC capacities is substantially lower and mainly into the MtA route, which is based on domestic waste-based feed as well as imports of green methanol. The production shift is also reflected in the feedstock supply costs which are in the current decade at about 31 bln \in per year. While the temporary shift to ethane and the initial shift to the cheaper waste-based routes (see Fig. 6) even reduces cost, in the second decade after 2035 feedstock costs increase again to 30 bln € per year, which is mainly due to the costs of embedded hydrogen from electrolysis for the non-fossil feedstocks. After 2045, a significant increase of imports of non-fossil methanol and naphtha feedstock leads to a value of 53.9 bln € per year in annual feedstock costs, which is >70 % over the current

level. The same trend is also reflected in the average costs of the final products which more than doubles over the scenario, from today $577 \notin$ per t to 1191 \notin per t. The split of costs shows that feedstock costs are dominating the picture in all years with shares in overall costs in a range of 80 % and more. Second are CAPEX and energy costs. While CAPEX is increasing over time, energy costs increase significantly from the current to the next decade and remain relatively stable afterwards.

Underlying this general trend, however, are major changes in HVC production routes, carbon feedstock and energy supply, resulting in very different cost increases for different HVCs. The main reason is that the new production routes have often strongly diverging yield structures which leads to over-proportionally high cost increases for some products such as benzene, toluene and butadiene. Fig. 8 shows that more standard HVCs such as ethylene and propylene display price increases of 30 to 40 % between 2020 and 2050, both with a peak in 2040. Para-xylene remains stable due to its low absolute demand and available excess flows and its price even massively decreases between 2040 and 2050 as it can be produced efficiently via the MtA route which is needed after 2040. On the other hand, butadiene, benzene and toluene show massive increases in marginal supply costs by factors of 5 to 10 between 2020 and 2050. The reason for this increase is that the very cost efficient non-fossil MtOroute yields none of these products. Butadiene can be supplied from steam cracking based on pyrolysis oils, but its volumes are limited as it requires clean polyolefin waste and yields only little BTX. This means that very expensive MtA routes need to be invested after 2040 to secure the supply of aromatics. Their yields, however, remain poor and their production can be increased only with the acceptance of high excess para-xylene volumes that, however, might be pushed into a "green" gasoline market (if existent). The developments of MtA plants with higher benzene and/or toluene yields would clearly be a relief for this bottleneck.

As the polymer demand is exogenously given it is per se inelastic in our analysis. As a consequence, the scenario shows an equilibrium situation on the supply side where costs nearly equal revenues. This is not the case for the two waste-based routes, but even for those waste purchase cost could increase up to levels that result in a cost-revenue parity.

However, MtA plants should be considered the most uncertain investment in the scenario, as they require a specific policy framework to enforce defossilisation, together with continued demand for benzene and toluene derivatives. Economic incentives alone are unlikely to be

⁴ Revenues have been calculated based on marginal supply cost.

 $^{^5}$ DAC: Direct Air Capture of CO₂. We assume, that the price of imported methanol from sweet spots for renewable electricity production will be set by methanol from DAC-based CO₂ and H₂ from water electrolysis as their availability is hardly restricted.



Fig. 7. Cost and revenue situation for non-fossil HVC plant operators in 2040 and 2050. Source: own figure.

Table 3

Financial key performance indicators. Source: own calculations.

	[unit]	2016–2025	2026–2035	2036–2045	2046-2055
Overnight invest (HVC supply)	[Bill. EUR]	-	5.6	34.3	10.8
Mean annual capex ^{*)}	[Bill. EUR/a]	-	0.6	4.1	5.2
Mean annual feedstock cost (incl. hydrogen)**)	[Bill. EUR/a]	31.4	20.2	30.0	53.9
Mean annual energy cost ^{**)}	[Bill. EUR/a]	2.4	3.9	4.3	4.2
Mean annual other opex	[Bill. EUR/a]	0.3	0.1	0.2	0.1
Mean annual transport cost ^{***)}	[Bill. EUR/a]	0.6	0.5	0.5	0.5
Mean specific polymer supply cost	[EUR/t polymer]	577	519	726	1191

*) Only for HVC production and without accounting of existing assets.

**) Sales of by-products are subtracted.

****) Costs include the transport of feedstock, HVC and intermediates.



Fig. 8. Marginal HVC production cost in the core scenario. Source: own figure.

sufficient. The other major uncertainty is the use of green naphtha in steam crackers. If the use of butadiene can be significantly reduced by shifts in the demand portfolio and/or if the use of biomass can be focused on butadiene production, the use of green naphtha will likely be very limited.

5.2. The future of the ARRRA region in the scenario

The final part of the results section analyses the impact of a defossilisation scenario on the ARRRA meta-cluster. This cluster consists of a number of sites (see above) linked via strong pipeline infrastructure connections that are represented in the model (see SI for documentation). The cluster does not form a separate model entity, but is analysed as an aggregate of the sites it contains. We analyse possible investment foci and ask how strong the future market position of the ARRRA sites could be and what kind of infrastructures would help to encourage defossilisation and keep up value added in the region.

The overall indicators for the ARRRA region with regards to investments and HVC production are not too different in the main scenario compared to the rest of Europe. However, there are some important differences that are useful to understand and which may have implications to the future robustness of this meta-cluster.

5.2.1. Investment

In the core scenario, the ARRRA can attract MtO investments of the order of 5 million tonnes per year by 2050, representing 42 % of total European capacity, mainly located in the ports of Antwerp and Rotterdam. This result is robust as it is confirmed by a sensitivity, where we assumed uniform energy prices across Europe (see Section 3 and Fig. 5 in the SI). The German sites are assumed to bear higher electricity prices compared to the sites in the Netherlands and Belgium and therefore they attract very few MtO investments, but in return they keep more steam cracker capacities (Fig. 9).

Investments in the MtA plants are limited to the harbours for cost reasons, as MtA require additional methanol imports from the world market and the liquid MtA products (aromatics) can easily be transported in product pipelines or by ship on the River Rhine.

In Section 2 we showed, that the ARRRA is particular unique in its high proportion of engineering plastics and polyurethane foams. These polymers require significantly more additional energy input on top of feedstock. In the ARRRA, the average steam intensity is 3.6 GJ/tonne of polymer, compared to an average of 2.8 GJ/tonne in the EU27+3. Today, chemical steam cracking by-products like methane or fuel oil are theoretically sufficient to meet this demand if burned, but with new HVC production lines coming on stream with higher conversion efficiencies, the ARRRA will run out of by-products to meet its steam demand in the long term. 55 % of all ARRRA polymer-related steam demand can be traced back to polyurethane production alone, which is therefore also most exposed to competition with renewable-rich regions in the world. The closure of BASF's relatively new TDI plant in Ludwigshafen at the beginning of 2023⁶ may be interpreted as an early indicator in this direction. Therefore, new ways of climate neutral and cheap steam generation are essential for this region more than for others to keep up these production lines operating with their high value added. Hybrid steam supply systems could do the job combining cheap electricity in times of high electricity infeed with firing by-products that cover the rest of the time. This can be supplemented with more efficient production pathways, e.g. by chemical recycling of benzene derivates like polyamide 6 and 6.6 or polyols.

A second competitiveness issue analysed is the performance of the ARRRA if there are demand shocks. As explained in the supplementary information (Section 3.2) we carried out stress tests to check the

performance of sites when the production of a single polymers is cut by 25 %. These cases should not be interpreted as a general economic crisis, but rather as normal market imbalances where the capacity in the production system is not optimally matched to the demand structure. To-day's simulated situations are displayed on the left side of Fig. 10. The dots indicate the situation with the price differences for electricity and natural gas between member states of the EU27 and UK as well as Norway according to Eurostat's energy price statistics for big consumers. The triangles show the modelled mean utilisation rate with uniform energy prices all over Europe.⁷ Today's actual situation is likely to be in between indicating a superior competitive situation for the ARRRA.

The right-hand side of Fig. 10 illustrates the 2050 situation: The dots show the dynamics if the ARRRA has to bear higher prices for (renewable) electricity in the future compared to other regions in Europe like Spain, Portugal, France or the Nordic countries. The merit order would clearly be different from today's situation where the Netherlands have the lowest natural gas and also low electricity prices for industry. In 2050, the ARRRA's competitive situation within Europe in our scenario is however still slightly better compared to the average of the rest of Europe, in particular for non-commodity plastics.

The case of uniform prices for electricity (and heat) in Europe reveals the competitive advantage of the ARRRA due to horizontal integration. Here, the competitive advantage is stronger than in the case with price differences. A regulated uniform European industry electricity price as advocated by the German chemical industry could therefore help the ARRRA. On the other hand, flexibility in electricity use could also help to drive down the actual average price companies have to pay and thus align electricity bills throughout Europe without the political instrument of a regulated price.

Simulation results for uniform energy prices support the hypothesis that a higher horizontal integration promotes higher plant utilisation rates. However, the ARRRA meta-cluster does not outperform the rest of Europe in the demand shock cases: the weighted mean total production reduction effect counting all 10 different demand shock cases is about 2 % for both regions. The additional hypothesis of a possible outperformance of a more deeply integrated cluster in the event of shocks can thus not be supported by the modelling results.

Within the ARRRA cluster, the hinterland sites (without own harbours) with their continued operation of steam cracking reliant on naphtha would face stronger economic risks compared to the port clusters as the economic performance of the green naphtha steam cracking route is highly dependent on butadiene revenues (see Fig. 7). Butadiene represents a small fluctuating market with a strong connection to one single demand sector, i.e. the tyre industry.

5.2.2. Possible infrastructure implications

There are two commodities that are likely to gain in transport volume: methanol and propylene. Methanol related infrastructure adjustments could include the retrofitting of the liquid oil product pipeline from Rotterdam to Ludwigshafen in order to be capable to transport methanol batches. Repurposing of crude oil pipelines following refinery closures is another option to open up cheap import opportunities for the Cologne and the Gelsenkirchen/Marl (Emscher-Lippe) clusters. In such a case the hinterland could even attract new non-fossil MtO plants (or even methanol-based refineries).

Propylene's transport volume rise is due to the yield structure of the MtO process, where the yield structure can only be steered to a limited extent towards ethylene or propylene. The propylene yield is in every case significantly higher than for the currently dominating naphtha

⁶ https://www.basf.com/global/en/media/news-releases/2023/02/p-23-13 1.html.

⁷ The uniform energy prices lead to several equivalent solutions of the optimisation problem and thus to model artefacts. To eliminate these, two cases were created: One case in which ARRRA has marginally cheaper energy prices and one case with marginally more expensive ones. The triangles show the respective mean value from both cases.



Fig. 9. HVC plant capacities in the ARRRA in 2050. Source: own figure.



Fig. 10. Polymer plant utilisation rates per polymer type in case of demand shocks in 2020 and 2050. Source: own figure.

steam cracking. In addition, the overall yield increases when the product structure is shifted towards propylene [19]. With regard to propylene infrastructure, there has been a long discussion in the region about closing the gap in the pipeline network between Geel/Meerhout and Cologne (via Geleen), which could indeed help the meta-cluster to better cope with temporary plant outages. The stress test analysis revealed that pipelines are in some of the demand reduction shock cases more occupied as they offer additional flexibility (see SI).

6. Conclusions

A scenario for petrochemicals in which the EU achieves a completely non-fossil feedstock by 2050 is technically feasible but would likely require a significant change not only in the feedstock base, but also in the HVC-producing plants. Due to polymer "losses" in the overall plastic stock (via trade, littering etc.), carbon losses in the recycling processes and the still growing demand for plastics, the potential contribution of carbon recycling is limited and "new" carbon will be continuously needed to feed the system, which could come from biomass or from synthetic feedstock based on CO_2 from direct air capture. Such a shift means that classical fossil based HVC production technologies will be phased out after 2030 and 2040 respectively and be replaced by nonfossil routes. Here, the MtA technology was identified as a bottleneck. Industrial scale MtA plants are not available today. To commercialise the technology, it would be necessary to improve the BTX yield and shift the yield spectrum towards benzene. In particular, because the demand structure is an input and thus inflexible in our model, defossilisation leads to a doubling of polymer production costs, but with huge differences for marginal production costs among polymers. However, disproportionate price increases will lead to changes in demand and production recipes that are not fully captured in our model.

The main driver for identified cost increases are the feedstock costs,

and value added from bulk polymers in the chemical parks may remain quite stable. One exemption, however, is the waste treatment and recycling sector where additional investments are required and may thus generate additional value added. To incentivise the shift from fossil to non-fossil feedstocks, which involves significant investment needs and rising feedstock and energy costs, significant levels of taxes on the use of fossil carbon, or equivalent measures such as subsidies or quotas for green feedstocks are needed. The ETS alone with its focus on end-of-life emissions will not be able to incentivize a feedstock revolution. With the assumed development of carbon tax levels, strong shifts do not occur in our model until the late 2030s, with levels of ± 200 per tonne of CO₂ equivalent in 2040 and a ban on the use of fossil carbon in the last model decade (2046–2055).

From a policy perspective, the finding that a carbon tax on feedstock as the core driver, together with a strategic adjustment to defossilisation and renewable energy supply, makes the transition to non-fossil basic chemistry possible at moderate additional costs for the raw materials, is encouraging. However, the fact that the feedstock transition requires a substantial carbon feedstock tax of \notin 200 per ton and above, and only starts after 2030 with a take-off around 2040 in our scenario, suggests that strong policy and possibly additional measures may be needed to bring about the non-fossil transition even earlier.

For the ARRRA meta-cluster its current competitive advantages of low energy costs and high flexibility due to strong infrastructural links will be challenged in a defossilised scnerio. At least for the aromaticsbased production that has been a focus of the cluster so far and probably also an important source of income. Particularly the cluster's current strength in these speciality plastics might suffer from the strong cost increases for benzene and toluene and the high energy intensity of the respective polymerisation steps. The latter is an additional disadvantage, as the cluster's cost advantage in fossil feedstock will diminish and may turn into a disadvantage in renewable energy costs.

However, there are strategies that ARRRA can use to adapt. These include repurposing its infrastructure, which can even increase resilience. Also, by adapting to fluctuating energy supplies (e.g. by making by-product upgrading and hybrid steam supply solutions more flexible), the ARRRA could offset the potential energy cost disadvantage it faces compared to regions such as Spain, Portugal or Sweden. Even more than for the EU as a whole, it seems crucial for the transnational ARRRA cluster to proactively adapt to the changes that defossilisation will bring. Our findings point to potential strategies that need to be actively pursued by the companies at different stages of the plastics value chain, as well as infrastructure providers and relevant governments.

Given the very complex and interconnected nature of the European petrochemical industry and its associated value streams, our model naturally has some important limitations that need to be taken into account when interpreting our results and that lead to further research questions for subsequent analyses. First, the interaction between petrochemical production and refining is simplified in the model. This is mainly relevant for medium-term developments and less so for longerterm developments, as we expect refineries to be phased out in the future, making this interaction much less relevant. But new-built green refineries could offer synergies in the future as well and accelerate the feedstock transformation, be it abroad or in Europe. Second, demand response to changing cost structures is not included in the model and is only partially covered by the iteration. As discussed above, this misses a very relevant part of the system that will certainly respond to changes in material costs induced by the feedstock transition. Third, there may be novel production processes that are not relevant or discussed today because they do not offer an advantage in today's fossil dominated cost structures. However, if the large cost differentials we find occur in the industry, such technologies may emerge and be implemented, leading to new options for system reconfiguration that may be underestimated by the model. Fourth, we were not able to fully explore the potential share of biomass as a feedstock in our analysis, as the use of biomass in the model runs was focused on overcoming bottlenecks rather than

competing with methanol from DAC. This can be accepted due to the general scarcity of waste biomass, but it is important to take this limitation into account, especially when comparing results with other studies. Finally, the model has limited external trade with the rest of the world. Such trade opportunities, as well as international competition, provide further flexibility to the system, and in particular to coastal locations, which can also influence system change. A European production system as outlined in this paper would require a trade regime that prevents continued fossil imports on all stages of the production chain.

The lack of incentives to create negative emissions remains a significant obstacle to defossilisation in the petrochemical industry. Companies aiming to comply with climate-neutral production often prioritise the continued use of fossil feedstocks combined with CCS in chemical parks and plastic waste treatment. However, this approach raises critical questions about its long-term feasibility and effectiveness in achieving deep decarbonization. Future research should therefore focus on assessing the availability of crude oil for feedstock purposes and its implications for achieving climate protection targets [20]. This includes examining the risks of dependency on fossil resources in scenarios where CCS deployment faces economic, technical, or temporal constraints. At the same time, the defossilisation of the plastics sector offers a promising pathway to generate negative emissions when coupled with CCS. To fully realize this potential, further investigation is needed into strategies for the simultaneous implementation of CCS and defossilised feedstock. This dual approach represents a significant challenge under current policy frameworks, as the availability of CCS can easily disincentivise investment in defossilisation. Research is needed to explore how policy instruments can be redesigned to align incentives, ensuring that both pathways can develop in parallel and support each other in driving the petrochemical sector toward genuine climate neutrality.

Further research can not only explore the limits of our approach but should also cover inner-company value chains and portfolio adaption or the wider socio-economic system, as the chemical industry and the energy system consist of different actors, some of which are large multinational companies, including the major oil companies. This diversity of interests and policies will also have a significant impact on the future development and success of the transition to climate neutrality in Europe and therefore needs to be taken into account as well.

CRediT authorship contribution statement

Clemens Schneider: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Max Åhman:** Writing – review & editing, Writing – original draft, Validation, Supervision, Conceptualization. **Stefan Lechtenböhmer:** Writing – review & editing, Writing – original draft, Supervision, Project administration, Funding acquisition, Conceptualization. **Mathieu Saurat:** Visualization, Software, Resources, Conceptualization.

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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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at 10.1016/j.egvcc.2024.100173.

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