

Contents lists available at [ScienceDirect](www.sciencedirect.com/science/journal/09213449)

Resources, Conservation & Recycling

journal homepage: www.elsevier.com/locate/resconrec

Detailed modelling of basic industry and material flows in a national energy system optimization model

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ARTICLE INFO

Keywords: Energy system modelling Industry Material flows Recycling Net-zero emissions Techno-economic pathways

ABSTRACT

National energy system models are often ill-equipped to examine the interconnections between material and energy systems, and the tradeoffs between energy or material use of limited resources are left unaddressed. An adapted energy system model (IESA-Opt) combined with a revised dataset, including 22 new material flows, 33 new processes, and revisions to existing processes, broadens the range of solutions. We show that including additional detail in the major energy-intensive material production sectors has a significant impact on the results of a net-zero emissions scenario for the Netherlands. . The result is different optimal technology investment pathways compared to the previous scenario, and total system costs that are 0.8 % lower over the time horizon. The results highlight the value of explicitly including detail on energy-intensive material and industry in analyzing interactions between sectors – particularly waste, chemicals and fuel production – and points to improvements in energy system modelling for industry.

1. Introduction

Climate change is the greatest environmental challenge of our time, and the industrial sector is a critical piece of that challenge. According to the IPCC, current international commitments under the Paris agreement are insufficient to limit global average temperature rise to 1.5 ◦C, making it likely that this threshold will be exceeded unless further action is taken to reduce emissions [\(Shukla et al., 2022;](#page-16-0) [Rogelj et al. 2015](#page-16-0)). Globally, industry accounted for 28 % of final energy consumption and 24 % of anthropogenic greenhouse gas emissions in 2019 ([IEA 2022](#page-15-0); [Shukla et al. 2022\)](#page-16-0), and emissions from industry have been growing faster since 2000 than the emissions from any other sector ([Shukla et al.](#page-16-0) [2022\)](#page-16-0).

Meeting the Paris agreement target requires reaching net-zero greenhouse gas emissions by 2050 or earlier [\(Shukla et al. 2022](#page-16-0)). Within that transformation, greenhouse gas emissions linked to the industrial sector are particularly difficult to address because of a few unique challenges.

First, growing consumption of industrially produced materials magnifies the scale of the challenge, as demand increases and global standards of living rise. Global material intensity has been growing at a faster rate than GDP per capita since 2000, and plastic demand in

particular has grown rapidly [\(Shukla et al. 2022](#page-16-0); [Stegmann et al. 2022](#page-16-0); [Zheng and Suh 2019](#page-16-0)). Greenhouse gas emissions from the production of materials more than doubled from 1995 to 2015, from 5 GtCO₂e to 11 GtCO₂e globally ([IRP 2020\)](#page-15-0). In a scenario assuming convergence of material consumption rates, [Krausmann et al. \(2018\)](#page-15-0) find that global annual material extraction would more than double by 2050. In addition to challenges posed by the growth outlook, the industrial sector often operates with long investment cycles, and industrial equipment can have long effective lifetimes. Further, many industrial processes require high temperature heat, which limits the potential energy sources that are available. Finally, the use of fossil hydrocarbons as feedstock leads embedded carbon in products to be emitted at the end of product lifetimes, often after they are transformed and cross national borders, making these carbon flows difficult both to track and to regulate.

Even without including non-CO₂ greenhouse gases, net-zero $CO₂$ emissions scenarios for the industrial sector are difficult to achieve, and only possible with a combination of strategies from energy and material efficiency, renewable energy and material sources, circularity, new production processes (including electrification), and other abatement technologies, applied across value chains [\(Shukla et al. 2022\)](#page-16-0). Because of conversion losses and inherent process emissions, $CO₂$ -neutral energy alone is insufficient to reach emissions targets. Reaching net zero will

<https://doi.org/10.1016/j.resconrec.2024.107617>

Available online 17 April 2024 Received 30 August 2023; Received in revised form 25 March 2024; Accepted 6 April 2024

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require a transformation of the materials and products provided by industry, to break the cycle of extractive resource use leading to greenhouse gas emissions and environmental degradation.

Industry makes up 18 % of GDP, 24 % of final energy, and 30 % of greenhouse gas emissions in the Netherlands ([World Bank 2022](#page-16-0); [CBS](#page-15-0) [2022\)](#page-15-0). Retaining jobs and a comparatively high share of basic industry is a priority for Dutch policymakers ([EZK, 2020\)](#page-15-0), making the challenges of the industrial transition particularly relevant for national policymaking.

Circularity is therefore a particular focus in Dutch policymaking, both as a climate mitigation strategy and to address other environmental and economic issues. Dutch plans explore extended producer responsibility for products, product design to prevent waste, market incentives, and circular procurement in order to reduce raw materials usage, substitute raw materials, extend product lifetimes, and improve processing of waste and recycled materials ([Ministerie van Infra](#page-15-0)[structuur en Waterstaat, 2023\)](#page-15-0). The EU also aims to increase recycling and re-use of products to benefit the economy and the environment through a series of actions including a single-use plastic ban, new labelling requirements, and new recycling targets [\(European Commis](#page-15-0)[sion, 2020](#page-15-0)). Despite these ambitions, quantitative measurements of circularity and its potential remain limited even in these extensive policy documents. Improvement of modelling for circular economy and climate mitigation is specifically named as an action point in the EU plan.

This paper proposes a model and dataset that better accounts for materials in the industrial sector. This methodology allows us to use optimization modelling to evaluate tradeoffs between material and energy, and build improved scenarios for the future of Dutch industry.

2. Background

Energy system optimization models are designed with a variety of approaches, to answer questions with different geographical, temporal, and sectoral scopes. A number of challenges are identified in the literature for energy system optimization models, including increasing temporal and spatial resolution, broadening geographical coverage, increasing sectoral disaggregation, quantifying uncertainty, and increasing transparency (Plazas-Niño et al. 2022; [Aryanpur et al. 2021](#page-15-0)). Large, bottom-up optimization models used to build long-term scenarios must balance detail with computational capacity and data availability ([Pfenninger et al. 2014\)](#page-16-0). Global- and national-scale models often leave out new technologies, material efficiency, and circularity options in favor of a broader scope, and are less detailed than bottom-up sector models ([Shukla et al. 2022\)](#page-16-0). A recent review of modelling tools concludes that material recycling is insufficiently considered, and that both fields would benefit from coupling energy system and material flow models [\(Kullman et al. 2021](#page-15-0)).

Though other modelling methodologies, such as stochastic or multicriteria decision-making modelling, may also be used to develop relevant long-term scenarios for industry, optimization models are often used for policy analysis ([DeCarolis et al. 2017](#page-15-0)). Using an optimization approach in this analysis allows us to efficiently examine materials in the context of a net-zero emissions scenario and to make relevant comparisons with other studies.

Pfenninger et al. recommend the development of nimble models to deal with specific questions, as new challenges evolve in the energy system ([Pfenninger et al. 2014](#page-16-0)). Indeed, many existing national-level energy models are inadequate to answer questions about the dramatic transformations of the industrial sector that will be needed to achieve net-zero emissions by 2050. As the focus in policymaking shifts from a supply-oriented, incremental approach to a more drastic reimagining of the energy system, the questions being asked of energy system models are changing, and the range of policy measures and solutions being considered are broadening [\(Pye et al., 2021;](#page-16-0) [Fodstad et al. 2022](#page-15-0)).

Further, more data has become available on the end-use sectors¹ and many organizations are moving towards open-source data and code.

In order to address these new demands in the context of Dutch industry, we aim to improve the energy system optimization modelling tools available to represent this critically important, difficult-to-abate sector. As new value chains begin to link feedstock with alternative energy sources, and new materials and products are developed to replace the fossil-based, emissions-intensive versions, these new relationships must be represented within energy system models at a similar level of detail to the conventional, fossil value chains in order to evaluate the use of limited non-fossil resources for energy and material purposes [\(Pye et al., 2021](#page-16-0))

The interactions between materials and the energy system are extensive and should be included in energy systems modelling. Technology investment decisions are based on many factors, including availability and costs of both energy and material inputs. Energy and climate policies can even enhance the interconnectedness of material and energy choices; for example, the proposed Carbon Border Adjustment Mechanism (CBAM) would apply carbon pricing to goods and materials entering the EU from countries with less restrictive environmental regulation, supporting energy-intensive materials production within the EU with low-emissions technologies ([European Commission,](#page-15-0) [2023\)](#page-15-0). Using material flow analysis, [Krausmann et al. \(2017\)](#page-15-0) estimate that "convergence of material stocks at the high level of industrial countries is not compatible with the global climate change mitigation target agreed in Paris," illustrating the need for net-zero emissions scenarios that take into account material use.

There is a growing body of literature regarding the material, and particularly mineral, requirements of a future energy system ([Tokimatsu](#page-16-0) [et al. 2017;](#page-16-0) [Boubault et al. 2018](#page-15-0); [Tokimatsu et al. 2018](#page-16-0); [Månberger and](#page-15-0) [Stenqvist 2018;](#page-15-0) Capellán-Pérez et al. 2020; International Energy Agency [2021;](#page-15-0) [van Oorschot et al. 2022;](#page-16-0) [Hund et al. 2023](#page-15-0)), bringing to light the effects of changing energy demand on mineral requirements. Our focus is on a distinct but related topic: materials produced and used in large-scale, energy-intensive industrial sectors in the Netherlands, and their impacts on investments in the energy system. This requires similar characterizations of material flows but considers material needs when designing the energy system, rather than as an ex post calculation, allowing us to identify areas where material choices constrain or influence technology investments in the energy system.

The goal of this research is to adapt an existing energy system optimization model to better represent the industrial sector and material flows within major energy-intensive production processes, looking broadly at interactions with the energy system. We increase the level of granularity in the industrial sector, and make explicit the modelling of key materials and technologies that are used to produce and transform them. The results from the adapted model will be compared to previous results to evaluate the utility of the adaptations and the potential for new insights into investments and choices in the energy system.

3. Methodology

To address these questions, we have selected the IESA-Opt model, a national-level energy system model of the Netherlands with high technological detail and flexible temporal, sectoral and spatial granularity, using a linear programming (LP) least-cost optimization approach ([Fig. 1\)](#page-2-0). The model generates a set of linear equations based on the given data, then solves the linear problem, finding a set of investments and

¹ In the Netherlands, for example, the MIDDEN project (PBL Netherlands [Environmental Assessment Agency, 2024\)](#page-16-0) has gathered detailed techno-economic information on many of the largest industrial sites and sectors, and the AIDRES project provides similarly detailed information about industrial technologies and emissions at high geographical resolution across Europe [\(VITO, 2024](#page-16-0)).

operation variables that minimize the objective function (total discounted system costs) subject to given constraints (See [Appendix A](#page-8-0)). The scope of IESA-Opt is national, without a direct link to European or global models; however, the exogenous demand sector activity levels and commodity prices have been derived from the JRC's POTENCIA scenarios, and electricity prices have been derived from Europe-wide scenarios from the COMPETES model (Sanchez Diéguez et al. 2021).

IESA-Opt was selected for several reasons. It already contained a relatively high level of detail on industry and the power system, compared to many other models. It has proven utility in analyzing the Dutch energy system and industrial sector (Sánchez Diéguez et al. 2021; Sánchez Diéguez et al. 2022; Martinez Gordón et al. 2021). Its flexibility is also an advantage; database-driven inputs allow the user to easily make changes to the assumptions and structure of the model. The model itself, as well as the software and necessary solvers, is freely available with an academic license.

However, the combination of explicit material flows included in the optimization and highly granular sector, product and technology representation goes beyond the scope of national energy system optimization models that we are aware of (Capellán-Pérez et al. 2020; Fattahi [et al., 2020;](#page-15-0) [Prina et al. 2020;](#page-16-0) [Wiese and Baldini 2018;](#page-16-0) [Fleiter et al.](#page-15-0) [2018;](#page-15-0) [Scheepers et al. 2022a](#page-16-0); [PBL 2019;](#page-16-0) [ETSAP 2023](#page-15-0)). To fill that gap, changes to the techno-economic dataset, constraints and post-processing of IESA-Opt are required. These amount to straightforward changes to the database and code that could be easily adapted to other models, but represent a different way of thinking about energy systems modelling, and requires additional data.

Material flows can generally be treated similarly to energy carriers, as inputs and outputs to technologies or processes, when constraints are implemented to ensure thermodynamic laws are respected, and labels are correctly applied in results. Data inputs are formatted for IESA-Opt, but because public data are used, could be adapted for other models. With these additions, the model optimizes not only the energy system, but an interconnected system of energy and materials, and accounts for how material inputs influence energy supply and technology investment choices.

3.1. Techno-economic data

Additional data inputs were needed to represent relevant technologies and flows of materials, such as inputs and outputs of polymer production and waste disposal. These technologies, processes, intermediate materials, final products and fuels, currently represented in the model

either implicitly or in an aggregated manner, have been added to the database as exogenous parameters.

Material additions include carbon-containing materials and feedstocks for the current Dutch energy system, but also potentially imported or purchased materials such as plastic waste, steel scrap, or pig iron. Even if not directly used for energy purposes, they can compete with energy carriers to supply carbon to a material production process (plastic waste) or influence the choice of process technology (such as steel scrap). The focus is on the most energy- and emissions-intensive materials in Dutch industry, rather than rare minerals or materials used in renewable energy technology. Technologies currently at a lower technology readiness level, as well as additional combinations of technologies and alternative fuels/feedstocks are also included (see [Appen](#page-9-0)[dix C](#page-9-0) for list of additions). The full dataset used to create the reference scenario for this paper is available on GitHub.

The main criteria for inclusion were:

- 1. Significance to Dutch industry;
- 2. Availability of techno-economic data; and
- 3. Links with energy use and emissions in the Netherlands.

These criteria led us to focus primarily on the most energy- and emissions-intensive sectors; chemicals is by far the most significant in the Netherlands ([CBS 2024a,](#page-15-0) [2024b](#page-15-0)) and site-level public data is available from the MIDDEN project [\(PBL 2024](#page-16-0)) (See [Appendix C\)](#page-9-0).

The additional material, technology, and energy carrier data gives the model flexibility to meet final demand with different process routes, such as by importing intermediate products (in the case of direct reduced iron or scrap metal) or by using waste products (in the case of polymers). For example, where previously, intermediate chemical production levels were fixed, they are now linked to final demand for polymers and chemicals. There are also additional possibilities in combining fuels and feedstocks in the chemicals sector, and recycling of polymers to material, feedstock and energy is made explicit. Similar datasets could be used in other energy system models to characterize the industrial sector and its main material flows.

3.2. Constraints

Because IESA-Opt treats material and energy flows interchangeably, no changes to the optimization objective function were needed. The user defines which energy carriers and materials are included within the model, and the categories of these flows are determined only by labels.

Note: The optimization is performed over the full time horizon with perfect foresight and flexible time resolution. The scenarios presented in this paper are presented with five-year time steps and hourly resolution for electricity, daily resolution for gaseous energy carriers, and annual resolution for all other energy carriers and systems. Outlined in dotted lines are the revised components compared to the previous version of IESA-Opt. [Fattahi et al. \(2021\)](#page-15-0) describe the model's development. However, the model has been revised to consider materials as an additional set of commodities, to which different constraints can be applied. Energy can only be converted to material (and vice versa) with specified processes, in which the appropriate units and calorific values are taken into account. Commodities which can be used for material or energy purposes, such as mixed plastic waste which can be incinerated or further sorted, may be converted between material and energy with "dummy" processes with no cost or conversion losses.

While in most cases, the underlying equations for energy and materials are the same, there are several constraints which require materials to be treated differently; for example, in many cases, energy carriers may be produced and sold or exported beyond the exogenous demand (for example, waste heat is produced even when there is no demand, and surplus fuels produced beyond domestic demand may be exported at the market price). For materials, however, it is assumed that supply must exactly equal demand $(Eq. (1)$ replaces $Eq. (2)$. This avoids the production of surplus carbon-containing materials to artificially avoid emissions, and is more appropriate for a materials in a partial equilibrium model lacking representation of commodity markets.

$$
\sum_{t} u_{t,p} AP_{t,am,p} = V_{am,p} \tag{1}
$$

$$
\sum_{t} u_{t,p} A P_{t,a,p} \geq V_{a,p} \tag{2}
$$

where $t =$ index of the set of all technologies

 $p =$ index of the set of all modelled time periods

 $a =$ index of the set of all activities

am = index of the set of all material conversion activities; subset of *a*

 $u_{t,p}$ = technology *t* in period *p*

 $AP_{t,ap}$ = balance of inputs and outputs of activity *a* to a technology *t* in a period *p,* and

 V_{ap} = exogenous required output of an activity *a* in a period *p*

3.3. Post-processing

Adaptations to post-processing facilitate comparison between energy and material flows, costs, and units. In order to do this, labels are applied to explicitly categorize and identify material uses. This allows the user to track materials flowing through the energy system.

4. Results

The reference scenario describes a pathway for a net-zero emissions Dutch energy system without major restructuring of the economy or policy efforts to push specific technologies or energy carriers. Output growth remains in many industrial sectors, and behavioral shifts play a minor role, represented by, for example, a plateau in aviation transport demand and declines in minimum fuel exports after 2030. See [Appendix](#page-9-0) [B](#page-9-0) for a summary of scenario assumptions.

The result is a scenario where fuel exports continue to dominate final energy use, oil and oil products are phased out, while natural gas (with carbon capture) maintains a large role, and wind, solar, and nuclear energy scale up through 2050. $CO₂$ shadow prices peak in 2040 at around ϵ 120/tCO₂-eq, while annual total system costs increase by about 70 % from 2020 to 2040 and remain high in 2050 (Fig. 2).

After implementation of the revisions discussed above, the optimization, for a scenario with the same emissions constraints and demand drivers, led to results that differ in subtle but significant ways. Total system cost was reduced by about 0.8 % over the time horizon, when revenues for energy exports are included. The inclusion of more detailed

Fig. 2. High-level indicators illustrate the system-level effects of model revisions on the reference scenario, including reduced total system cost in 2040, increased CO2 shadow price in 2050, and an increase in both import costs and export revenues.

Note: Primary energy figures exclude energy for export and imported energy carriers. The optimization is based solely on costs, but in the above figure, export revenues are subtracted from the total system costs, and represent assumed market prices for exported energy carriers (material exports are excluded).

representation of material flows in the industrial and waste disposal sectors broadened the possible outcomes in these sectors, and also induced shifts beyond the industrial sector to different pathways for the refining and conversion sectors more broadly. Some sectors saw cost increases, due to increased retrofitting costs and more realistic process parameters.

The most notable changes are in the management of municipal waste. In addition to providing more detail on recycling processes and waste materials, the new database also harmonizes mass and energy units for municipal waste. Based on the updated database, advanced collection and sorting techniques, represented at an aggregated level, become cost-competitive by 2030, and lead to a supply of mono-stream plastic waste which can be processed more efficiently. By 2050, about 1 Mt of plastic waste that would otherwise be incinerated is used for mechanical recycling back to polymers, resulting in the production of about 0.45 Mt additional recycled polymers (beyond what already results from conventional separation and recycling processes). In the previous reference, about the same amount of waste was gasified to produce syngas. This is about 12 % of municipal waste (by mass) in 2050. For comparison, the Plastics Transition Agenda estimates that about 250–300 kt plastics were recycled via mechanical recycling back to polymers in 2015, and projected an increase to 1 Mt by chemical and mechanical recycling by 2030 [\(Transitieteam Kunststoffen, 2018\)](#page-16-0). Data regarding current and future waste composition and future technology costs and availability are particularly uncertain, introducing uncertainty into the optimization results. With additional data on emerging technologies for more selective waste separation and improved recycling routes (including for polymers that are not currently recycled at large scale, such as polyvinylchloride), the model could perhaps go beyond the 2030 estimates to a more ambitious scenario.

The previous model assumed constant calorific values for waste streams, regardless of separation steps. Thus, the energy carrier "municipal waste" had an LHV (lower heating value) of 5.5 GJ/t, both before and after a part of the stream was used for gasification.

Gasification requires a purer stream of higher energy content materials, so in reality, the remaining municipal waste stream should have a lower energy content. Additionally, the model could use waste energy beyond the required waste mass. While at average system level, these values were a reasonable approximation, the technology choices did not represent realistic uses of municipal waste streams (Fig. 3).

Changes in waste processing, in combination with additional process options in the basic chemistry sector, lead to changes in technology investments for high value chemicals (HVC) production. Recycling plastic waste is more attractive from a cost perspective than gasification of waste into syngas, particularly in later years. Increasing capacity for mechanical recycling back to polymers from 2030 onwards leads to reduced ethylene and propylene production. By 2050, about 175 kt ethylene production (about 9 % of total ethylene demand) is avoided because of material recycling processes that directly produce polymers. In addition to the lower production levels needed for HVC, technology investments for virgin high value chemicals production also shift. Bioethanol dehydration becomes an attractive option for ethylene production from 2030 onwards. In the short term, recycling takes on a smaller role than in the previous reference; this is a result of the more specific recycling processes with realistic potential based on explicit links to polymers, and because demand reduction is not included alongside recycling as part of the same technology option. The overall result is capital investment costs that are 4 % lower over the time horizon than in the previous model.

Because of the changes in the waste sector – both recycling over gasification, and harmonized mass and energy units – the biomass gasification value chain (biomass to syngas, syngas to methanol, methanol to synthetic fuels) displaces the waste gasification value chain (waste $+$ hydrogen to syngas, syngas to Fischer-Tropsch fuels) in the revised reference scenario. The additional availability of methanol, enabled by reductions in hydrogen use for waste processing via gasification, also leads to a greater role for methanol-to-olefins in the basic chemistry sector, further reducing the role of naphtha cracking,

Fig. 3. Mass, energy, and carbon flows in the waste disposal sector in 2050, from municipal waste (blue) to combined heat and power (CHP) with carbon capture (green), gasification (orange), and recycling (red), with sorting steps in shades of blue in the revised model Note: In the previous model, waste is assigned an average CO₂ emissions factor of 106 kgCO₂/GJ (for all streams), and is treated as fully biogenic. The new version considers waste partially biogenic (with varying shares of fossil carbon per stream). Technology options are the result of constrained least-cost optimization, chosen from the available options. See $Appendix E$ for more details about available options.

particularly in 2050 (Fig. 4).

Electrified steam cracking plays an intermediate role in the previous reference scenario, which disappears in the revised reference. In conventional steam crackers, fuel gas (generated in the cracking furnace from the feedstock) is used to fuel the cracker. However, in the case of alternative fuels such as electricity or hydrogen, this fuel gas is still generated inherently in the process but not used as fuel, and needs another outlet. In the previous scenario, this was assumed to be used onsite, and thus only net energy requirements were included. By explicitly including the full feedstock and fuel gas streams, we find that electrified cracking is less attractive due to the "higher" (compared to the previous assumption) energy and feedstock requirement. See [Appendix D](#page-12-0) for energy balance. Excess energy outputs can be used to meet fuel demand within the sector or elsewhere in the energy system. Availability and scalability of new technologies in this sector, such as electrified cracking and CO2 capture, and required infrastructure, creates uncertainties with regards to the optimization results; these results warrant additional investigation.

These shifts also lead to changes in investment decisions in the refining sector, due to shifts in price and availability of heat and captured $CO₂$. Synthetic fuels production makes up the majority of the refining sector's output by 2050, in both reference scenarios. In the previous model, by 2050, almost 600 PJ of syngas, primarily from biomass gasification, was used for synthetic fuels production, driven by demand for synthetic kerosene for aviation. In the revised reference scenario, the 2050 total is even higher, reaching about 750 PJ. Fischer-Tropsch routes become the dominant processes for synthetic kerosene production in both references, but account for all of the synthetic kerosene output in 2050 in the new reference compared to about 65 % in the previous reference, displacing methanol-to-fuels processes. The result is a reduction in the net hydrogen input to the refining sector ([Fig. 5\)](#page-6-0), reducing the overall imports of hydrogen at the national level and increasing biomass imports.

In addition to shifting towards biomass imports, the new configuration of the refining and chemicals sectors in the revised reference also leads to a greater surplus of synthetic naphtha than in the previous reference. Minimum fuel exports are an exogenous assumption scenario; the Dutch refining sector is assumed to reduce its trade surplus for most fuels, phasing out exports of naphtha and road fuels, while increasing its net export position on kerosene ([Appendix B\)](#page-9-0). However, the results suggest a potential role for flexible fuel production processes, in a scenario where demand for sustainable kerosene for export increases while domestic use of naphtha feedstock declines. The most cost-competitive option based on the current model structure is to export the surplus synthetic naphtha as well (Fig. 6), while shifting the domestic basic chemistry industry away from naphtha-based steam cracking towards alternative process routes.

Other industrial sectors also see changes; the new, disaggregated structure of the paper and board sector allows for inclusion of technologies which apply to specific segments. The results show a 100 % replacement of conventional drying with microwave drying for board production by 2040, while the paper sector continues with traditional production processes. In the previous reference, compressed refining, an innovative, pre-commercial papermaking technology, was deployed for almost all capacity; this does not appear in the new result because it is not applicable to all product categories, and because energy savings compared to conventional technologies were revised to more realistic values. Overall, costs from the paper and board sector are about 12 % lower over the time horizon compared to in the previous model.

In the iron and steel sector, given the high costs of imported raw materials, no changes are observed in the technology choices compared to the previous version of the model. By 2040, the full production of the Netherlands (7 Mt/year) is produced via direct reduction with natural gas. In 2050, hydrogen replaces natural gas, and biomass replaces coal as a reducing agent. This trajectory is slower than the announced plans of the sector, but in line with the planned technology pathway.

Fig. 4. Ethylene production, shown by process and feedstock, shifts away from steam cracking in the new version of the model towards bio-based routes and methanol-to-olefins, while recycling takes a more realistic role compared to the aggregated recycling and demand reduction from the previous model. Note: The reference scenario already includes considerable reduction in demand for ethylene production in the Netherlands (50 % reduction by 2050), based on structural changes in the economy in both the Netherlands and abroad. Recycled and avoided material in the previous model included both mechanical recycling and reductions in demand via material efficiency and reduced consumption elsewhere in the value chain.

Fig. 5. Sankey diagrams, Dutch fuel production 2050.

Note: Sankey diagrams represents inputs to fuel production (oil products and natural gas and their bio- and synthetic equivalents and substitutes), and their use as final energy carriers. Use of other energy carriers in end-use sectors is not shown above. Values have been rounded.

Fig. 6. Total final energy consumption (including feedstock and excluding exports) in 2050 is reduced in the revised model compared to the previous model reference scenario, particularly for the industrial and waste disposal sectors.

By 2050, the model is already highly constrained by ambitious emissions targets, and domestic carbon-neutral energy carriers are limited (offshore wind is limited to 87 GW, and solar to 70 GW, in 2050, and total domestic biomass to just over 200 PJ/year). Available resources may be reallocated, but, especially in later years, there is little freedom in changing the overall mix of fuels, particularly given the assumed growth in Dutch industry and fuel exports. The notable exceptions are imported hydrogen and biomass, which can be imported virtually without limit at relatively low prices (ϵ 4.2/kg H₂ and ϵ 35/GJ woody biomass in 2050). This assumption is subjected to sensitivity analysis, with results presented in [Appendix F](#page-14-0).

The new reference solution sees slightly reduced hydrogen use in 2050 (about -100 PJ) compared to the previous model, offset by increased biomass and biofuels imports, because the most difficult to abate sectors (shipping, aviation, and basic chemistry) still require hydrocarbons (with carbon of biogenic or circular origin), and biomass gasification to syngas becomes more competitive than synthesis of captured carbon and hydrogen. In the revised reference, we see about 150 PJ (~5 %) less final energy consumption in 2050 overall, spread across energy carriers, occurring mainly in the sectors where major revisions to the model were made.

5. Discussion

The comparison of previous model results with an updated scenario demonstrates that including more detailed representation of material flows and industrial technology can lead to significantly different and more relevant results. Notably, technology investments in the basic chemistry sector and waste sectors shift away from steam cracking, and recycling of waste to polymers becomes more competitive than recycling to feedstocks.

Changes in the waste disposal sector are robust to several key uncertainties (availability of biomass imports and technology cost for mechanical recycling, see [Appendix F\)](#page-14-0). While choice of recycling route is highly context dependent, results confirm other researchers' findings that recycling of material is preferable from a climate mitigation

perspective to waste incineration, when economically and technically feasible, and that oil and feedstock prices are key determinants of the choice between waste disposal options ([Scheepers et al. 2022a](#page-16-0), [Gar](#page-15-0)[cia-Gutierrez et al. 2023](#page-15-0)), necessitating integrated analysis with the rest of the energy system. Models like the one developed for this analysis can help policymakers understand linkages between material and energy systems and between different sectors of the economy. Continuing to expand the model database to include circular strategies beyond recycling, such as demand reduction, lifetime extension, and reuse of products or components, will help in further examining these linkages.

Some other aspects of the energy system look similar despite revisions to the model structure and database. These results are aligned with other studies of the Dutch energy system, in which domestic wind and solar resources are deployed to their maximum potential, while significant carbon-neutral energy imports continue and industrial activities shift to new process routes [\(Scheepers et al. 2022b](#page-16-0); [Netbeheer](#page-16-0) [Nederland 2023\)](#page-16-0). It is precisely because of the limited flexibility in the system that technology pathways in specific industrial sectors become more relevant. Results from the OPERA model also suggest that biogenic carbon from biomass gasification plays an important role in the chemicals sector, though recycling deployment is based on exogenous assumptions [\(Scheepers et al. 2022a](#page-16-0)). Other analyses confirm in broad strokes the ability of the sector to transform itself to use much larger quantities of carbon-neutral energy, but do not present sub-sector technology choices [\(PBL 2023](#page-16-0); [Netbeheer Nederland 2023](#page-16-0)).

Because exogenous assumptions about activity levels and international trade have a large impact on the results, it is important to continue to explore alternative, transformative scenarios. This new version of IESA-Opt can be used to question fundamental scenario assumptions and to test the implications of different assumptions about the future of the Dutch economy, particularly focusing on materials as suggested by [Krausmann et al. \(2017\).](#page-15-0) The surplus of synthetic naphtha that emerges while biomass and biofuel imports increase is an example; though trade assumptions are unable to capture the rebalancing of global trade and of industrial activities, this model can provide insights into which industrial structures are more and less logical based on the interlinkages of energy and material in industry.

6. Conclusion

Based on comparison with results from a previous version of the model, it is clear that adding details in material flows and industrial processes leads to different technology investment decisions, such as the phase-out of most steam cracking capacity by 2050, investment in additional Fischer–Tropsch fuels production, and recycling of plastics back to material, as well as different energy trade patterns, including reduced imports of hydrogen, increased exports of naphtha and increased imports of biomass. Neglecting the reconciliation of mass and energy for the waste disposal sector leads to unrealistic results; the results of this analysis provide an improved picture of the tradeoffs between energy and material use of end-of-life polymers which is internally consistent in mass and energy terms.

Findings from previous research are also confirmed; in a net-zero emissions scenario, sourcing synthetic or biogenic hydrocarbons is an important constraint on sustainable production in the chemicals and refining industries, in the Netherlands and internationally [\(Sanchez](#page-16-0) Diéguez 2022; [Scheepers et al. 2022a\)](#page-16-0). Our findings also highlight where current assumptions about future product output and exports may be out of alignment with climate ambitions and resource availability, necessitating additional research into alternative visions and scenarios for the future structure of Dutch industry.

The results also raise broader questions about the robustness of the model to represent transformative change. Circularity, material efficiency and demand reduction options have not been comprehensively considered here, and their further inclusion, planned in future work, could loosen the constraints on the system [\(Alwood et al. 2010](#page-15-0)).

Systematic evaluation of the uncertainties inherent in key parameters would also be valuable [\(Yue et al. 2018](#page-16-0)).

This model can also be linked with other tools to explore transformative scenarios – for example, considering alternative production scenarios, climate policy frameworks, and impacts of the energy and materials system beyond national borders. The connection of energy systems modelling with more detailed tools to track material flows would improve insights into the most effective long-term emission reduction strategies given the available resources (Kullmann et al. [2021\)](#page-15-0).

More broadly, the results point to the need for the energy system modelling community to integrate a more detailed view of material production and use into models, beyond rare minerals. This model begins to address gap by correcting inconsistencies and broadening options available in a highly constrained system. Future work should take this a step further, integrating material flow analysis with energy systems modelling to better account for material efficiency and circularity, which have a large potential for future emissions reductions and remain underrepresented in national models ([Alwood et al. 2010;](#page-15-0) [Kullmann](#page-15-0) [et al. 2021;](#page-15-0) [Shukla et al. 2022\)](#page-16-0).

CRediT authorship contribution statement

Kira West: Writing – review & editing, Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Data

Appendix A: Objective function in IESA-Opt

The objective function, *f*, of IESA-Opt is the sum of discounted total system costs over the modelling time horizon, and reads

$$
f = \sum_{p,l} \alpha_p \left(\sum_{jp} IL_{i,p,p} CRF_t \left(i_{t,p} IC_{t,p} + \sum_{i_i,j_j} r_{i_i,j_j} RC_{i_i,j_j,p} \right) + s_{t,p} FC_{t,p} + u_{t,p} VC_{t,p} \right)
$$

where $t =$ index of the set of all technologies

 p *,* jp = index of the set of all modelled time periods

 a_p = social discount factor in period *p*

 $I\!I_{t,p,ip}$ = binary matrix parameter for investment lifetime of a given technology, such that

 $IL_{t,p,p} = 1$ if technology t is within its lifetime in period p after investment in period jp and $IL_{t,p,p} = 0$ if technology t is not within its defined lifetime in period *p* after investment in period *jp*

 $IC_{t,p}$ = investment cost of a technology in a period

 $RC_{t_i,t_j,p}$ = retrofitting cost from one technology t_i to another technology t_j in period *p*

 $FC_{t,p}$ = fixed operational costs of a technology in period *p*

 $VC_{t,p}$ = variable costs of a technology in period *p*

 $CRF_t =$ capital recovery factory for a technology *t*

 $i_{t,p}$ = investments in a technology in period *p*

 r_{t_i,t_j} , p = retrofitting from one technology t_i to another technology t_j in a period *p*

 $s_{t,p}$ = stock (installed capacity) of a technology *t* in period *p*

 $u_{t,p}$ = use of a technology *t* in period *p*

Note on retrofitting costs:

Compared to previous versions of IESA-Opt, the assumed costs for technology retrofits are revised in the new version of the model, to better account for differences between conventional technologies and processes and their replacements. Rather than considering only the difference in capital costs, an additional cost is assumed to account for required changes in operating parameters, auxiliary equipment that may not be present in the greenfield costs. Similarly, recovery of costs with early decommissioning is removed, as it is assumed that salvage values are limited, given the dramatic transformations occurring in the energy system. These considerations are particularly important in the industrial sector, where major changes to process equipment are required in order to meet emissions targets.

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curation, Conceptualization. **Toon van Harmelen:** Writing – review & editing, Validation, Supervision, Conceptualization. **Vinzenz Koning:** Supervision, Methodology, Conceptualization, Validation, Writing – review & editing. **Gert Jan Kramer:** Conceptualization, Methodology, Supervision, Validation, Writing - review & editing. André Faaij: Conceptualization, Funding acquisition, Methodology, Project administration, Supervision, Validation, Writing – review $\&$ editing.

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.

Data availability

The model version used for this analysis is available at https:// github.com/IESA-Opt/IESA-Opt-N. Refer to version 5.3. Databases for the described scenarios are also available on GitHub.

Acknowledgements

This work was supported by TNO (The Netherlands Organisation for Applied Scientific Research) and Utrecht University.

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Appendix B: Key input parameters to the reference scenario in the new and revised model versions

Note: Description of the scenario assumptions from the previous model for other sectors can be found in Appendix B of Sanchez Diéguez et al. 2021. Ethylene and propylene production in the revised model refer to ethylene and propylene additional to what is used within the Netherlands as input for polymers. Paper and board are aggregated in the previous version of the model. Exports of fuels refer to fossil naphtha, liquid fuel for vehicles, or kerosene, or their bio-based or synthetic equivalents. No price premium is considered for exports of alternative fuels, but emissions from exported fuels must meet the same targets as domestic emissions, including net-zero by 2050. Mvkm = million vehicle kilometers, Mt = megatonnes, PJ = petajoules, $GJ = gigajoules$.

Appendix C: Summary of additions to industrial, waste, and refineries sectors in the new version of IESA-Opt

(*continued on next page*)

(*continued on next page*)

(*continued*)

(*continued on next page*)

Notes: Additions to the database are shown in bold italics above. This list does not include on-site heat & electric utilities in industry (except where these are integrated with process equipment). The remainder of the industrial sector is modelled in an aggregated manner, as "machinery – industry," "other ETS chemicals," "other ETS industry," and "other non-ETS industry." Products indicated with an asterisk (*) were previously used as activity drivers, and are now intermediate products whose production is driven (fully or partially) by demand for final products. Processes indicated with a double asterisk $(**)$ have been revised for consistency with new or other existing processes. Some additional notes on the modelling of steam cracking processes and waste separation and recycling are given in Appendix D and E. The shares are based on national energy and emissions statistics [\(CBS 2024a](#page-15-0); [CBS 2024b](#page-15-0)), to the closest possible matching sector.

These additions are not comprehensive. Some material flows have been excluded. For example, calcination of limestone and carbonate clays is a significant source of carbon emissions in the global cement sector, but these materials are almost exclusively processed outside the Netherlands. Iron ore and steel scrap, on the other hand, are explicitly modelled because of the major role of iron and steelmaking within the Netherlands in terms of energy and emissions, and because their costs directly impact the choice of technology and energy carrier for processes inside the model scope. Based on the available statistics for energy and emissions, the explicitly modelled industrial sectors cover roughly 80 % of 2022 energy use (including feedstock use of energy carriers) and 90 % of industrial greenhouse gas emissions ([CBS 2024a; CBS 2024b](#page-15-0)). All of the explicitly modelled sectors have some coverage in the publicly available MIDDEN database [\(PBL 2024](#page-16-0)) and reports (see table above), which is the primary source where available, supplemented with other sources.

The full dataset and its sources is available on GitHub ([https://github.com/IESA-Opt/IESA-Opt-N\)](https://github.com/IESA-Opt/IESA-Opt-N). Refer to version 5.3. Note that relevant data from the previous industrial sector modelling in IESA-Opt is also described in Sanchez Diéguez et al. 2022.

Appendix D: Modelling of steam cracking processes

Alternative feedstocks for steam cracking remain, for the most part, pre-commercial and input data is therefore relatively uncertain. To what extent blending of different feedstocks is possible, how it will affect efficiency or product quality, and the impacts of the use of alternative feedstocks in combination with alternative fuels are all worthwhile research topics in their own right. The table below (Table D.1) includes the assumptions regarding energy and material inputs and outputs for each of the modelled technologies. The general assumption is that feedstock requirements remain constant compared to conventional naphtha steam cracking when alternative biogenic or synthetic feedstocks are used. Energy requirements for crackers with alternative fuels, and corresponding outputs of fuel gas are derived from literature.

Because defining processes with flexible inputs would require a mixed-integer linear programming approach, which would increase the computational requirements and require a more limited scope of the overall model, each combination of fuel and feedstock is modelled as a separate technology. The model allows for retrofits between the technologies with an assumed retrofit cost, where other data is not available, of the difference of the costs in the two technologies plus 10 % of the original technology's capital investment cost. The same approach applies for the retrofit of carbon capture equipment. Note pyrolysis oil is treated differently from other feedstocks; it may be blended with fossil naphtha at a fixed ratio (10 % mass basis); this feedstock is based on pyrolysis of mixed municipal plastic waste. It differs from synthetic naphtha, which is based on Fischer-Tropsch or methanol-to-fuels processes.

Table D.1

Steam cracking technologies, inputs and outputs.

Sources: IESA-Opt database; [Oliveira and van Dril 2021.](#page-16-0)

Appendix E: Modelling of waste separation and recycling processes

Municipal waste as defined explicitly in [Appendix C](#page-9-0) refers to additional recycling beyond the current recycling programs in the Netherlands, and the volumes are based on the waste that is currently sent to waste incineration facilities (typically waste-fuelled combined heat and power (CHP) units). The remainder of the current recycling sector, including recycling from construction waste or recovered plastic and glass from deposit programs, is included in the "other industry" category and represented in an aggregated way, as in energy statistics.

All waste is treated as having an average biogenic content, which leads to an average CO_2 factor of 106 kgCO₂/GJ, which is assumed to be constant over time [\(Netherlands Enterprise Agency 2022\)](#page-16-0). There is considerable uncertainty in the content of future waste streams, however, and their biogenic content will also be dependent on technology investment and operation choices. Additional data is needed to address the limitations of this approach in future model versions, and scenarios can be created that more explicitly investigate the effects of changes in municipal waste.

Possible routes for treatment and recycling of municipal waste are shown in the figure below. Fig. E.1.

Fig. E.1. Multiple mechanical and chemical recycling routes are available for polyethylene, polypropylene, and polyethylene terephthalate in IESA-Opt.

Appendix F: Sensitivity to key input parameters

Many of the input parameters to such optimization scenarios are uncertain. The effects of these uncertainties warrant additional, dedicated research using a systematic approach as recommended by [Yue et al. \(2018\).](#page-16-0) Assumptions about availability and price of imported fuels and feedstocks are particularly crucial to understanding the possibilities – and limits – for the industrial sector. Given the importance of imported energy in the scenarios, the assumption of freely available imported biomass from the Americas is tested in a sensitivity analysis. Reducing the available biomass for import from outside Europe leads to an increase in CO₂ prices, and crucially, an increase in hydrogen imports. As European biomass imports are lower-cost than imports from the Americas, the full potential of European biomass imports (300 PJ/year) is used in all cases. The system requires imports of carbon-neutral energy, and in the revised model, biomass is more cost-effective than hydrogen. Increasing potential for biomass imports from the Americas beyond about 250 PJ/year does not make a meaningful difference in 2050 CO₂ prices or hydrogen imports (Fig. F.1).

Notably, the results for the waste disposal sector, in which mechanical recycling to material is deployed rather than gasification, are derived mainly from the reconciliation of mass and energy units in waste resources, and thus remain unchanged in scenarios with stricter constraints on biomass imports. Though biomass gasification can replace waste gasification, the shift away from waste gasification is not driven by low-cost imported biomass.

Imported H2 2050 Imported biomass, Europe 2050 Imported biomass, Americas 2050 CO2 price 2050

Fig. F.1. Reduced biomass import supply from the Americas increases the need for hydrogen imports and increases carbon prices by 2050.

A sensitivity case was also performed on the capital and fixed operating costs of mechanical (polymer to polymer regranulation) recycling technologies. The deployment of this technology occurs even in extreme scenarios where the CAPEX and OPEX are much greater. The shift away from gasification of waste towards this type of recycling is a result of the improvement of the representation of the energy content per unit of mass of waste plastics and other waste materials, rather than by changes in the technology costs for these particular technologies. By recycling waste plastics back to polymers, avoided costs in the whole supply chain of basic organic chemistry outweigh even large increases in CAPEX and OPEX. In the case where mechanical recycling (regranulation) costs are dramatically increased, depolymerization and dissolution technologies enter the solution.

Change in CAPEX and OPEX for mechanical recycling

Mechanical recycling/regranulation Depolymerization and dissolution Change in 2050 system cost

Large increases in CAPEX and OPEX for mechanical recycling have limited effect on total system cost.

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