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Original article

The effects of industrial policymaking on the economics of low-emission technologies: The TRANSid model

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ABSTRACT

Basic materials such as steel, cement, aluminium, and (petro)chemicals are the building blocks of industrialised societies. However, their production is extremely energy and emission intensive, and these industries need to decarbonise their emissions over the next decades to keep global warming at least below 2 °C. Low-emission industrial-scale production processes are not commercially available for any of these basic materials and require policy support to ensure their large-scale diffusion over the upcoming decades. The novel transition to industry decarbonisation (TRANSid) model analyses the framework conditions that enable large-scale investment decisions in climate-friendly basic material options. We present a simplified case study of the cement sector to demonstrate the process by which the model optimises investment and operational costs in carbon capture technology by 2050. Furthermore, we demonstrate that extending the model to other sectors allows for the analysis of industry- and sector-specific policy options.

1. Introduction

The industrial processes used to produce basic materials over the last centuries are unsuitable for an economy with a net zero carbon footprint. Basic materials such as steel, cement, aluminium, and (petro)chemicals are the building blocks of industrialised societies; however, their production is highly energy and emission intensive. These four sectors constitute 45% of global energy and 70% of all industrial emissions [1]. These industries must implement decarbonisation over the next decades to maintain global warming well below 2 °C, preferably below 1.5 °C, as pledged by 193 signing parties in the 2015 Paris Agreement [2]. In the European Union (EU), the entire economy shall be climate neutral by 2050 [3], whereas some member states, such as Sweden (2017 Climate Act) and Germany (2021 Climate Law), are committed to decarbonisation by 2045.

This transition implies replacing the current emission-intensive conventional processes with novel climate-friendly technologies. Leading steel producers champion novel hydrogen-based direct reduced reduction processes [4], whereas the cement sector favours carbon capture and utilisation or storage (CCUS) options to reduce emissions to an absolute minimum. Pathways to a climate-friendly (petro)chemical industry include bio-based and hydrogen-based production processes combined with CCUS [5]. For all basic materials used, a higher share of recycling is expected [6]. However, low-emission industrial-scale production processes have not been commercialised for any of these materials. These technologies and other low-emission options are vital to any pathway towards climate neutrality, as described in domestic or global transition roadmaps [7]. Nevertheless, all low-emission solutions feature higher investment and operational costs than the current conventional processes [8], which poses the question, “How can these technologies become competitive?”. Moreover, some industrial equipment has a design life of up to 50 years [9], which implies that current investments in conventional technology within the EU might become stranded assets by the middle of the century.

Historically, basic materials are globally traded commodities with market prices that have converged since the Industrial Revolution [10]. Until now, national or geographically limited emission pricing mechanisms, such as the European emission trading system (EU ETS) or stricter emission limits for local producers, have been unsuccessful in fostering a transition toward low-emission basic material use. Price-sensitive consumers will buy basic materials on the global market if domestic production is more expensive, potentially increasing emissions or just displacing them. This effect is referred to as carbon leakage.

As shown in [11], to kick-start the transition of the basic materials sector and create domestic low-emission basic materials markets, a comprehensive policy package is needed beyond emission pricing mechanisms, including policies such as green public procurement (GPP), carbon contracts for differences (CCfD), an efficient carbon border adjustment mechanism (CBAM) and product carbon requirements (PCRs). Considering the sector-specific needs and different levels of technolog-

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ical readiness of low-emission options in each industry, it remains unclear which combination of policy options, implemented as industry-specific or horizontally across all sectors, can ensure that all emission-intensive industries complete their transition until 2050. Hence, the potential effectiveness of policy options and their interlinkages must be investigated to provide a market environment that fosters the diffusion of low-emission technologies and practices in the basic materials sector.

The importance of the industrial sector in the transition toward a low-emission or climate-neutral society has been reflected comprehensively in bottom-up energy system models. In 2011, Fleiter et al. [12] showed how industrial representation in energy demand models moved from an accounting approach based on external assumptions about technological transformation to linear optimisation models with technology options based on partial equilibrium in energy markets, considering demand and supply. Henceforth, energy system models have been increasingly used to evaluate cost-efficient global pathways to reduce emissions [13]. As shown in [14], the number of different system modelling approaches and the level of detail used to represent industrial transformation have increased significantly over time. However, energy system models remain primarily static, optimising investments and operations for a relatively short time (one year).

Because bottom-up energy system models are primarily suitable for reflecting horizontal policies such as global emission pricing, another approach might be required to reflect the industry-specific, instead of horizontal, nature of industrial policies [15]. Sector-specific transformations have been primarily evaluated using techno-economic assessments, which identifies the economic viability of technology options under consideration of operational and investment cost scenarios. Vogl et al. [16] identified potential energy, emission, and scrap price scenarios that can render hydrogen-based primary steel production competitive to conventional production processes. A two-part techno-economic assessment of various carbon capture options for the cement industry was presented in [17,18], whereas electrification options in the chemical industry were investigated in [19] by considering various energy price scenarios. Leeson et al. [20] captured the cross-sectional dimensions of transition in their techno-economic assessment of carbon capture employment for the global steel, cement, oil refining, and paper industries by considering industry-specific employment rates and costs until 2050. The results identified the top-down techno-economic boundary conditions for high carbon capture employment rates.

Additionally, policy-specific models have been used to address industrial transitions. Quantitative research on emission trading systems using various modelling approaches, such as agent-based models, system dynamics, artificial intelligence, optimisation, and statistical models, primarily focuses on the market dynamics of price formation and the trade-offs between goods included and excluded by the emission pricing system [21]. The potential effects of various policies on specific industries have also been investigated. Carbon pricing, combined with other policies such as grandfathering CO_2 allowances in the European cement sector, was investigated in [22] without considering structural changes to the industry. In [23], the effects of multiple policy options on the circular use of steel were investigated using a structural equation model, and a system dynamics approach was adopted in [24] to identify barriers to the transition of energy-intensive industries and subsequently propose policy options to address these barriers. The industrial transition challenge has been addressed from a policy perspective; nevertheless, the holistic effects of different policy options on industrial transformation beyond a specific sector have not been investigated.

Industrial transitions must be understood in a cross-sectoral context [14]. Existing modeling approaches are insufficient for understanding and analysing industrial transitions due to the importance of circular material use and the potential competition for available waste streams between industries [25]; the limited availability and optimal use of alternative renewable energy sources, such as electricity [26], biomass [27] and hydrogen [28]; and the emergence of horizontal policies [15], such as emission pricing without free allowances.

A literature review regarding the technological change in the emissions-intensive basic material industry, using both sector-specific techno-economic and energy system models, allows one to evaluate the factors that may result in technology adoption. However, previous studies failed to demonstrate how different industrial policy design options can result in technology adoption. Although existing studies regarding policy-orientated models consider the trade-offs between various policy choices, they typically disregard long-term technological changes across the industrial sector. Hence, our objective is to develop a modelling approach to identify policy design options that support the transformation of different industries.

Herein, a linear optimisation model, TRANSid, is introduced to investigate the effects of different policy designs on operational and investment decisions across different industrial sectors over the transition period toward a climate-neutral economy. Section 2, materials and methods, is followed by Section 3, theoretical model formulation. Subsequently, we demonstrate some of the model's functionalities using a simplified base case (Section 4) of investment decisions in the cement sector (Section 5). Finally, the insights and limitations of this case study are discussed in Section 6.

2. Material and methods

This section introduces the primary elements of the decision-making problem for industrial plant operators. We highlight the trade-offs between the decision variables used in the selected linear programming method to model investments and operational decisions under different policy scenarios.

2.1. Business case of basic material production

Most basic materials are commodities: non-alloy carbon steel constitutes approximately 80% of EU production [29]; five main categories of cement exist, with the majority represented by Portland and Portland composite cement [30]; and all products from the (petro)chemical sector are either natural gas or naphtha based [31]. Hence, most basic materials are traded based on global market prices, with slight to no differentiation or unique selling points. The business models of basic material producers are primarily cost driven. Some clients might be willing to pay premiums for low-emission products to support the transition toward a climate-neutral economy in the EU by 2050. However, this premium does not change the physical characteristics of basic materials or their cost-orientated business case. The relative premium payment, though, would have to exceed the difference between the production cost of low-emission basic material production and the market price for conventional basic materials. For a basic material producer to be competitive, it must minimise its investment and operational costs.

2.2. Investment decisions in the industry

Industrial processes in the basic material sector can be characterised by their long design life and high initial investment costs, ranging from 200 €/ton of annual capacity for kilns in the cement sector [32] to 4,200 €/ton of annual capacity for integrated aluminium plants [33]. The production of basic materials is no single-step process. Plants have numerous main process steps, operating in parallel in some industries and involving numerous auxiliary processes. Each piece of process equipment has a specific design life. Hence, gradually renewing equipment in existing facilities is more cost-effective than scrapping an entire plant or rebuilding a new greenfield facility. The production of low-emission basic materials typically requires processes that differ significantly from those used in conventional production facilities [34]. Plant operators must decide amongst reinvestment in conventional technologies (if feasible), the brownfield transformation of existing facilities into low-emission facilities, and the construction of new greenfield low-emission basic material production plants to produce virgin primary or secondary recyclate-based materials based on investment and expected operational costs.

2.3. Operational cost variables

Plant operators must bear the costs of operational feedstock (raw materials), energy, labour, and maintenance, with the weight of each cost position differing by industry. In 2017, energy costs constituted 11% of the sales price in the EU steel industry, 5% in the cement sector, and 4% in the organic chemical and fertiliser industry [35]. By reducing free allowances and phasing in CBAM within the EU ETS, conventional basic material production will be subject to increasing emission costs [36]. Hence, the cost of purchasing emission allowances is another operational cost element, whereas (if applicable) income from trading excess allowances can be an additional revenue stream.

2.4. Modelling assumptions

Based on the characterisation of the decision-making problem faced by industrial plant operators, we selected a linear programming approach that optimised the total cost of plant operations. To model the operational and investment decisions across the different basic material industries, we assumed that plant operators are price takers in all markets (energy, raw materials, EU ETS, and basic materials). Furthermore, plant operators make decisions to minimise their total expected costs over a long time horizon, which is equivalent to the economic design life of their investments, based on available knowledge about future market prices, technological availability, and technology costs. Hence, we modelled the expected investments of plant operators based on their perspectives on future markets, given the role of current and prospective industrial policy measures.

We performed a simplified case study of carbon capture options in the cement sector to demonstrate the general functionality of the model.

3. Theoretical model formulation

3.1. Sets and alias

$i,\ ii,\ iii$	Material/emission type	[clay, iron ore, CO2e, ...]
$e,\ ee$	Energy type	[electricity, thermal energy]
s, ss	Energy source	[electricity, natural gas, coal, ...]
$p,\ pp$	Production step	[1, 2, ... , N_p]
f	Plant level process	[1, 2, ... , N_f]
$t,\ tt, ttt$	Time step in years	[1, 2, ... , N_t]

3.2. Variables

$vCost$	Total costs over all p in all f at t	[€]
$vCostInstall_{p,f,t}$	Cost for installing p in all f at t	[€]
$vCostMaterials_{p,f,t}$	Cost of materials in p in all f at t	[€]
$vCostEnergy_{p,f,t}$	Cost of energy to operate p in all f at t	[€]
$vCostOperationalFix_{p,f,t}$	Additional costs to operate p in all f at t	[€]
$vCostEmissions_{f,t}$	Cost linked to emissions for f at t	[€]
$vCapacity_{i,p,f,t}$	Capacity to produce i with p in f at t	$[ton_{M/E}]$
$vNewCapacity_{i,p,f,t}$	New capacity added to produce i with p in f at t	$[ton_{M/E}]$
$vRetiredCapacity_{i,p,f,t}$	Retired capacity to produce i with p in f at t	$[ton_{M/E}]$
$vMaterial_{i,p,pp,f,t}$	Material flow i from p to pp in f at t	$[ton_M]$
$vMaterialProd_{i,p,f,t}$	Material i produced with p in f at t	$[ton_M]$
$vLegMaterialProd_{i,p,f,t,tt}$	Material i produced with p in f at t installed at tt	$[ton_M]$
$vEnergy_{e,s,p,f,t}$	Energy flow e to produce i with p in f at t	$[MJ]$
$vEnergyNeeded_{e,p,f,t}$	Energy flow e to operate p in f at t	$[MJ]$
$vEnergyRecovered_{e,p,f,t}$	Energy flow e recovered from p in f at t	$[MJ]$
$vEmissions_{i,p,pp,f,t}$	Emission flow i from p to pp in f at t	$[ton_E]$
$vEmissionProcess_{i,p,pp,f,t}$	Process emission flow i from p to pp in f at t	$[ton_E]$
$vEmissionsFuel_{s,i,p,pp,f,t}$	Fuel emissions flow i from p to pp in f at t	$[ton_E]$
$vCapEmissions_{i,p,f,t}$	Emissions i captured from p to pp in f at t	$[ton_E]$
$vCapBioEmissions_{i,p,f,t}$	Bio-emissions i captured from p to pp in f at t	$[ton_E]$
$vLegCapEmission_{i,p,f,t,tt}$	Emissions i captured from p to pp in f at t installed at tt	$[ton_E]$

3.3. Parameters

$InstallationCost_{p,f,t}$	Cost of installing capacity for p in f at t	$\left[\frac{€}{ton_{M/E}}\right]$
$MaterialCost_{i,t}$	Cost of purchasing i at t	$\left[\frac{€}{ton_M}\right]$
$EnergyCost_{s,t}$	Cost of energy source s at time step t	$\left[\frac{€}{MJ}\right]$
$OperationsCost_{p,t}$	Cost to operate p at t	$\left[\frac{€}{ton_{M/E}}\right]$
$EmissionCost_{i,t}$	Cost to emit i at t	$\left[\frac{€}{ton_E}\right]$
$DiscountRate$	Discount rate for calculating the NPV	[%]
$DesignLife_{p,f}$	Maximum design life of p in f	$[years]$
$PlantCapacity_{i,f,t}$	Maximum capacity to produce i in f at t.	$[ton_M]$
$MaterialDemand_{i,t}$	Total material demand of i to be met at t	$[ton_M]$
$MaterialNeed_{i,\ ii,\ p,t}$	Material of i needed to produce ii with p at t	$\left[\frac{ton_M}{ton_M}\right]$
$EnergyNeed_{e,p,t}$	Energy type e to operate p at t	$\left[\frac{MJ}{ton_{M/E}}\right]$
$EnergyExcess_{e,p,t}$	Off-heat e from operating p at t	$\left[\frac{MJ}{ton_{M/E}}\right]$
$EnergyMaxRestrict_{e,s,p,t}$	Technical restriction for energy source s in p at t	$\left[\frac{MJ}{MJ}\right]$
$MaxEnergyAltShare_{e,p,t}$	Maximum share of energy source s in p at t	$\left[\frac{MJ}{MJ}\right]$
$EmissionProcess_{i,p}$	Process emissions i caused when operating p	$\left[\frac{ton_E}{ton_M}\right]$
$EmissionFuel_{s,i}$	Fuel emissions i caused when using source s	$\left[\frac{ton_E}{MJ}\right]$
$BioEmissionFuel_{s,i,t}$	Share of bio-based emissions i using source s at t	$\left[\frac{ton_E}{ton_E}\right]$
$CaptureRate_{i,p}$	Share of emissions captured from i by p	$\left[\frac{ton_E}{ton_E}\right]$
$CaptureRange_{i,p,pp}$	Ability of p to capture emission I from pp	[0/1]

3.4. Objective function

The TRANSid model minimises the investment and operational costs across various plant operators in various industrial sectors over the entire time horizon of the transition (N_t), whereas industries are differentiated by the material type i determined by the production processes p at the plant/factory level f. Hence, the main objective function minimises the net present value (NPV) of installation, material, energy, fixed operational, and emission costs (Eq. (1)).

$$\min vCost[€] = \sum_{t}^{N_t} \frac{1}{(1 + DiscountRate[\%])^t} * \left[\sum_{f}^{N_f} \left[\sum_{p}^{N_p} vCostInstall_{p,f,t}[€] + vCostMaterials_{p,f,t}[€] + vCostEnergy_{p,f,t}[€] + vCostOperationalFix_{p,f,t}[€] \right] + vCostEmissions_{f,t}[€] \right] \quad (1)$$

This objective function is subject to various constraints.

3.5. Installation costs

The annualised installation cost related to each p is the sum of all annuities of newly installed equipment in t and all previously installed equipment *(tt)*. Constant annual annuities are calculated based on the total installation cost via the NPV approach (Eq. (2)).

$$vCostInstall_{p,f,t}[€] = \sum_{i}^{N_{ii}} \sum_{tt}^{N_{tt}} vNewCapacity_{i,p,f,tt}\left[ton_{M/E}\right] * InstallationCost_{p,f,tt}\left[\frac{€}{ton_{M/E}}\right] * \frac{(1 + DiscountRate[\%])^{DesignLife_{p,f}[years]}}{\sum_{a=1}^{DesignLife_{p,f}[years]} \frac{1}{(1+DiscountRate[\%])^a}},$$
$$\forall tt : t \leq t, \forall tt : t > t - DesignLife_{p,f}[years] \quad (2)$$

3.6. Operational costs

The first production step (*p = 1*) serves as material stock. All the material flows from this production step have an associated material cost (3). All external energy sources *s* have associated energy costs that may vary for different *t* (Eq. (4)). The general operational cost depends on the actual production volume for each *p* (Eq. (5)). Emission costs must be paid for atmospheric fossil emissions, excluding captured emissions. Meanwhile, profits can be achieved by capturing bio-based emissions (Eq. (6)).

$$vCostMaterials_{p,f,s}[€] = \sum_{i}^{N_i}\sum_{pp}^{N_{pp}} vMaterial_{i,p,pp,f,t}\left[ton_M\right] * MaterialCost_{i,t}\left[\frac{€}{ton_M}\right],\ \forall p:\ p=1 \quad (3)$$

$$vCostEnergy_{p,f,t}[€] = \sum_{s}^{N_s}\sum_{e}^{N_e} vEnergy_{e,s,p,f,t}[MJ] * EnergyCost_{s,t}\left[\frac{€}{MJ}\right] \quad (4)$$

$$vCostOperations_{p,f,t}[€] = \sum_{i}^{N_i} vMaterialProd_{i,p,f,t}\left[ton_M\right] * OperationsCost_{p,t}\left[\frac{€}{ton_{M/E}}\right] \quad (5)$$

$$vCostEmissions_{f,t}[€] = \sum_{i}^{N_i}\sum_{p}^{N_p}\sum_{pp}^{N_{pp}}\Big(vEmissions_{i,p,pp,f,t}\left[ton_E\right] - vCapturedEmissions_{i,pp,f,t}\left[ton_E\right] - vCapturedBioEmissions_{i,pp,f,t}\left[ton_{BE}\right]\Big) * EmissionCost_{i,t}\left[\frac{€}{ton_E}\right] \quad (6)$$

3.7. Capacity additions

Material production cannot exceed the capacity of the production step *p* (Eq. (7)). Capacity can change over time through capacity addition and retirement (Eq. (8)). The capacity retires when it reaches the end of its design life (Eq. (9)). The parameter $PlantCapacity_{i,f,t}$ is used to dimension plants *f* (Eq. (10)) with legacy capacities installed at *t=1* (Eq. (11)).

$$vCapacity_{i,p,f,t}\left[ton_{M/E}\right] \geq vMaterialProd_{i,p,f,t}\left[ton_{\frac{M}{E}}\right],\forall p:\ p>1 \quad (7)$$

$$vCapacity_{i,p,f,t}\left[ton_{M/E}\right] = vCapacity_{i,p,f,tt}\left[ton_{M/E}\right] + vNewCapacity_{i,p,f,t}\left[ton_{M/E}\right] - vRetiredCapacity_{i,p,f,t}\left[ton_{M/E}\right],\ \forall p:\ p>1,\ \forall tt:\ t=t-1 \quad (8)$$

$$vNewCapacity_{i,p,f,t}\left[ton_{M/E}\right] = vRetiredCapacity_{i,p,f,tt}\left[ton_{M/E}\right],\ \forall p:\ p>1, \forall t:\ t\leq N_t - DesignLife_{p,\ f}[years],\ \forall tt:\ t=\ t+\ DesignLife_{p,\ f}[years] \quad (9)$$

$$PlantCapacity_{i,f,t}\left[ton_M\right] \geq \sum_{p>1}^{N_p} vMaterialProd_{i,p,f,t}\left[ton_M\right],\ PlantCapacity_{i,f,t} > 0 \quad (10)$$

$$vCapacity_{i,p,f,t}\left[ton_M\right] = vNewCapacity_{i,p,f,t}\left[ton_M\right],\ \forall t:\ t=1 \quad (11)$$

3.8. Material flows

If a certain demand is defined for a material, then it shall be produced by the modelled industries because material production must be sufficient to satisfy the demand (Eq. (12)). The output material *ii* of each *pp* requires one or multiple input materials *i*, defined by the parameter $MaterialNeed_{i,\ ii,\ pp,t}$ originating from another *p* (Eq. (13)). Because one *p* can generate more than one output material *i*, the variable $vMaterialProd_{i,p,f,t}$ accumulates all production for each *p* (Eqs. (14)–(17)). For $vMaterial_{i,p,pp,f,t}$ to represent only feasible flows between different p's and the material stock (*p*=1), the flows must be restricted (Eq. (18)).

$$MaterialDemand_{i,t}\left[ton_M\right] \leq \sum_{f=1}^{N_f}\sum_{p=1}^{N_p} vMaterialProd_{i,p,f,t}\left[ton_M\right],\ MaterialDemand_{i,\ t}\left[ton_M\right] > 0 \quad (12)$$

$$vMaterialProd_{ii,pp,f,t}\left[ton_M\right] \leq \sum_{p=1}^{N_p} vMaterial_{i,p,pp,f,t}\left[ton_M\right] * MaterialNeed_{i,\ ii,\ pp,t}\left[\frac{ton_M}{ton_M}\right], MaterialNeed_{i,\ ii,\ pp,t}\left[\frac{ton_M}{ton_M}\right] > 0,\ \forall p:\ p>1,\ \forall pp:\ p<>p \quad (13)$$

$$vMaterialProd_{i,p,f,t}\left[ton_M\right] \geq\ vMaterial_{i,p,pp,f,t}\left[ton_M\right],\ \forall p:\ p>1,\ \forall pp:\ p<>p \quad (14)$$

$$vMaterialProd_{i,p,f,t}\left[ton_M\right] \geq \sum_{pp<>p}^{N_{pp}} vMaterial_{i,p,pp,f,t}\left[ton_M\right] \quad (15)$$

$$vMaterialProd_{ii,p,f,t}\left[ton_M\right] \leq MaterialNeed_{i,\ ii,\ p,t}\left[\frac{ton_M}{ton_M}\right] * \infty\left[ton_M\right],\ \forall p:\ p>1 \quad (16)$$

$$vMaterialProd_{ii,p,f,t}\left[ton_M\right] \leq \sum_{pp}^{N_{pp}} vMaterial_{i,p,pp,f,t}\left[ton_M\right],\forall p:\ p=1 \quad (17)$$

$$vMaterial_{i,p,pp,f,t}\left[ton_M\right] = \begin{cases} 0,\ \forall pp:\ p=1 \\ 0,\ \forall pp:\ p=p \\ 0, \forall p:\ p=1,\ MaterialCost_{i,t}=0 \end{cases} \quad (18)$$

3.9. Differentiation between material and emission flows

Both material and emission flows are particle-matter flows, *i*. Constraints (Eqs. (19)–(22)) are introduced to differentiate between both flow types. Legacy variables for materials and emissions refer to production in time step *t* with the equipment installed in previous steps *tt*.

$$vMaterialProd_{i,p,f,t}\left[ton_M\right] = \sum_{tt\leq t}^{N_{tt}} vLegacyMaterialProd_{i,p,f,t,tt}\left[ton_M\right],\ \forall p:\ p>1 \quad (19)$$

$$vCapturedEmission_{i,p,f,t}\left[ton_E\right] = \sum_{tt\leq t}^{N_{tt}} vLegacyCapEmission_{i,p,f,t,tt}\left[ton_E\right],\ \forall p:\ p>1 \quad (20)$$

$$vNewCapacity_{i,p,f,tt}[ton_M] \geq vLegacyMaterialProd_{i,p,f,t,tt}[ton_M] + vLegacyCapEmission_{i,p,f,t,tt}[ton_E], \forall p : p > 1 \quad (21)$$

$$vLegacyMaterialProd_{i,p,f,t,tt}[ton_M] + vLegacyCapEmission_{i,p,f,t,tt}[ton_M] = 0, \forall tt : t \leq t - DesignLife_{p,f}[years] \quad (22)$$

3.10. Energy flows

Similar to material and emission legacy flows, the legacy energy required for each production step refers to the energy flows required to operate older equipment at t (Eq. (23)). The actual energy flow ($vEnergy_{e,s,p,f,t}$) to p in plant f at t depends on not only the energy requirement but also on the type of energy consumed (electricity, thermal energy, or both) (Eq. (24)) and the maximum proportion of specific energy carriers that can be consumed (Eq. (25)). The latter is determined by the maximum proportion of biomass that certain processes can handle (Eq. (26)). The thermal-energy consumption of p results in excess heat specific to each p. This excess heat can be recovered to reduce primary energy consumption (Eqs. (27)–(28)).

$$vEnergyNeeded_{e,p,f,t}[MJ] = \sum_{i=1}^{N_i} \sum_{tt}^{N_{tt}} EnergyNeed_{e,p,tt}\left[\frac{MJ}{ton_{M/E}}\right] *(vLegacyMaterialProd_{i,p,f,t,tt}[ton_M] + vLegacyCapEmission_{i,p,f,t,tt}[ton_E]), \quad \forall tt : t \leq t \quad (23)$$

$$vEnergy_{e,s,p,f,t}[MJ] \leq vEnergyNeeded_{e,p,f,t}[MJ] * EnergyRestrict_{e,s}\left[\frac{MJ}{MJ}\right] \quad (24)$$

$$vEnergy_{e,s,p,f,t}[MJ] \leq \sum_{i}^{N_i} \sum_{t}^{N_{tt}} EnergyNeed_{e,p,tt}\left[\frac{MJ}{ton_M}\right] * EnergyMaxRestrict_{e,s,p,tt}\left[\frac{MJ}{MJ}\right] * (vLegacyMaterialProd_{i,p,f,t,tt}[ton_M] + vLegacyCapEmission_{i,p,f,t,tt}[ton_E]), \forall tt : t \leq t, \ EnergyMaxRestrict_{e,s,p,tt}\left[\frac{MJ}{MJ}\right] > 0 \quad (25)$$

$$\sum_{s}^{N_s} vEnergy_{e,s,p,f,t}[MJ] \leq MaxEnergyAltShare_{e,p,t}\left[\frac{MJ}{MJ}\right] * \sum_{s}^{N_s} vEnergy_{e,s,p,f,t}[MJ] * EnergyRestrict_{e,s}\left[\frac{MJ}{MJ}\right], \ EnergyMaxRestrict_{e,s,p,t}\left[\frac{MJ}{MJ}\right] > 0 \quad (26)$$

$$vEnergyRecovered_{e,p,f,t}[MJ] = \sum_{i=1}^{N_i} \sum_{tt}^{N_{tt}} EnergyExcess_{e,p,tt}\left[\frac{MJ}{ton_M}\right] *(vLegacyMaterialProd_{i,p,f,t,tt}[ton_M] + vLegacyCapEmission_{i,p,f,t,tt}[ton_E]), \ \forall tt : t \leq t \quad (27)$$

$$\sum_{s}^{N_s} \sum_{p}^{N_p} vEnergy_{e,s,p,f,t}[MJ] = \sum_{p}^{N_p} vEnergyNeeded_{e,p,f,t}[MJ] - vEnergyRecovered_{e,p,f,t}[MJ] \quad (28)$$

3.11. Emission flows

Emissions can originate from either process reactions or fuel consumption Eq. (29)). Process emissions are related to production step p and depend on the production level at t (Eq. (30)). The emissions from fuel consumption depend on the fuel type and the specific emission factors (Eq. (31)); these emissions are either released into the atmosphere or captured. The emissions captured inside f at t cannot exceed the installed capture capacity of p (Eqs. (32) and (33)), and are subject to the capture efficiency of the installed capture equipment p (Eq. (34)). Furthermore, emission capture depends on the type of equipment used to capture emissions from all or only one specific p of plant f (Eq. (35)). Some of the captured emissions can be of biological origin and are identified as such Eqs. (36)–(38).

$$vEmissions_{i,p,pp,f,t}[ton_E] = vEmissionProcess_{i,p,pp,f,t}[ton_E] + \sum_{s}^{N_s} vEmissionsFuel_{s,i,p,pp,f,t}[ton_E] \quad (29)$$

$$\sum_{pp}^{N_{pp}} vEmissionsProcess_{s,i,p,pp,f,t}[ton_E] = \sum_{ii}^{N_{ii}} vMaterialProd_{ii,p,f,t}[ton_E] * EmissionProcess_{i,p}\left[\frac{ton_E}{ton_M}\right] \quad (30)$$

$$\sum_{pp}^{N_{pp}} vEmissionsFuel_{s,i,p,pp,f,t}[ton_E] = \sum_{e}^{N_e} vEnergy_{e,s,p,f,t}[MJ] * EmissionFuel_{s,i}\left[\frac{ton_E}{MJ}\right] \quad (31)$$

$$vCapturedEmissions_{i,p,f,t}[ton_E] \leq vCapacity_{i,p,f,t}[ton_E] \quad (32)$$

$$\sum_{p}^{N_p} vEmissions_{i,p,pp,f,t}[ton_E] \leq vCapacity_{i,pp,f,t}[ton_E] \quad (33)$$

$$vCapturedEmissions_{i,pp,f,t}[ton_E] \leq \sum_{p}^{N_p} vEmissions_{i,p,pp,f,t}[ton_E] * CaptureRate_{i,pp}\left[\frac{ton_E}{ton_E}\right], CaptureRange_{i,pp,pp}[0/1] = 1 \quad (34)$$

$$vCapturedEmissions_{i,pp,f,t}[ton_E] \leq vEmissions_{i,p,pp,f,t}[ton_E] * CaptureRate_{i,pp}\left[\frac{ton_E}{ton_E}\right], CaptureRange_{i,pp,p}[0/1] = 1, \ \forall pp : p <> p \quad (35)$$

$$vCapturedBioEmissions_{i,pp,f,t}[ton_E] \leq \sum_{s}^{N_s} \sum_{p}^{N_p} vEmissionsFuel_{s,i,p,pp,f,t}[ton_E] * CaptureRate_{i,pp}\left[\frac{ton_E}{ton_E}\right] * BioEmissionFuel_{s,i,t}\left[\frac{ton_E}{ton_E}\right], \ CaptureRange_{i,pp,pp}[0/1] = 1 \quad (36)$$

$$vCapturedBioEmissions_{i,pp,f,t}[ton_E] \leq \sum_{s}^{N_s} vEmissions_{i,p,pp,f,t}[ton_E] * CaptureRate_{i,pp}\left[\frac{ton_E}{ton_E}\right] * BioEmissionFuel_{s,i,t}\left[\frac{ton_E}{ton_E}\right], CaptureRange_{i,pp,p}[0/1] = 1, \ \forall pp : p <> p \quad (37)$$

$$vCapturedBioEmissions_{i,pp,f,t}[ton_E] \leq vCapturedEmissions_{i,p,f,t}[ton_E] \quad (38)$$

Table 1
Materials required for production [18].

	(i to ii)
Clinker to cement	0.737
Gypsum to cement	0.050
Mineral additions to cement	0.213
Raw meal to clinker	1.600
Limestone ($CaCO_3$) to raw meal	0.770
Silica (SiO_2) to raw meal	0.140
Al_2O_3, Fe_2O_3, $MgCO_3$ to raw meal	0.090

4. Case study

The TRANSid model is designed to optimise investment and operations over several different industries by satisfying the material demand scenarios of i in the entire time horizon of the transition N_t as defined by $MaterialDemand_{i,t}$. However, for the following simplified base case, we only consider two legacy cement plants (f01, f02) (capacity: 1 Mt/year each) with the option to invest in new processes or install a new plant (f03) to satisfy a constant annual demand of 2 Mt/year between t01 = 2020 and t29 = 2050. The techno-economic data for the conventional production equipment and new carbon capture installations are based on academic sources (Tables 1–5 [5,17,18,37,38,38,39]).

Investment decisions are subject to material, energy, and emission price scenarios. Energy prices were assumed to be constant for all but hydrogen (prices declined logarithmically between 2020 and 2050) (Table 6 [17,40,41]). Electricity and hydrogen use do not cause direct emissions, whereas constant emission factors were assumed for fossil fuels. The materials were assumed to have constant prices for all t, which were adopted and adjusted based on Ref. [17] (Table 7). The kiln and precalciner generate process emissions due to the burning of limestone (Table 8 [17,38]). In the base case, only one linear emission price scenario was applied. Owing to the current system of free allowances in the EU ETS, the net emission price was set at 0 €/tCO_2 in 2020, which increased linearly to 250 €/tCO_2 until 2050.

5. Results

The following results were obtained by translating the mathematical formulation into a General Algebraic modeling System (GAMS) model, executed under release 34.2.0 using the IBM CPLEX solver (release 20.1.0.0) on an Intel Core i7–3770 @ 3.4 GHz (eight CPUs) and 32 GB RAM with an average run time of 27.52 s to obtain an optimal solution.

The results for the base case show that existing plants are being renovated instead of opting for new greenfield installations if future demand remains constant. Without emission pricing, the total cement production costs are 59.3 €/t cement at t01 = 2020 (Fig. 1). This value is approximately 30% higher than that estimated in [17]. This difference can be explained by the higher installation cost component subject to the NPV (Eq. (2)).

The emission reduction technology, namely monoethanolamine (MEA) carbon capture, is only installed at t10 = 2031 in both existing plants, although it is available from the time step t05 = 2024. This shows that the model only opts for its installation as soon as economically justifiable, owing to high emission prices of > 90 €/tCO_2 in 2031, to minimise the relative production cost per ton of cement. As soon as it becomes available, the LEILAC carbon capture technology was installed in both plants, even when the previously installed MEA technology had not reached the end of its design life. Here, the significantly lower energy costs of LEILAC justify the installation of additional equipment, even if the payable annuities for both technologies increase the installation cost component (Fig. 1). Fossil energy sources are used to satisfy the thermal energy demand of the cement kilns over the entire time horizon. Thus, the emission costs for non-capturable emissions remain constant until the final time step. Hydrogen use can only reduce fuel emissions (Table 6) and not process emissions, as shown in Table 8. Hence, the model will only consume hydrogen if carbon capture technologies are unavailable. Alternatively, high CO_2 prices that increase the cost of CO_2 emissions are not captured, owing to a capture efficiency below 100% (Table 4) or an emission limit, resulting in hydrogen and biomass use as fuel.

Table 2
Energy required for production.

Production step		$EnergyNeed_{e,p,t}$ MJ/ton (i)		Output (i)		Sources
		e = electric	e = thermal			
p02	Raw material handling	15	20	i04	Raw meal	[18,37]
p03	Raw mill	83	-	i05	Raw meal grinded	[18,37]
p04	Preheater	-	–600	i06	Clinker (preheated)	[5,38]
p05	Precalciner	-	2,219	i07	Clinker (precalcined)	[5,38]
p06	Kiln	119	1,479	i08	Clinker (hot)	[18,37,39]
p07	Cooler	-	-	i09	Clinker (cold)	[5]
p09	Cement mill	112	-	i13	Cement mixed	[5,18,37]
p10	Finishing/auxiliaries	35	-	i14	Cement final	[18,37]

Table 3
Design life and installation costs.

Production step		$DesignLife_{p,f}$ (years)			$InstallationCost_{p,f,t}$ (€/ton (i))		Sources
		New	f01	f02	Total	Annuity (f01/f02)	
p02	Raw material management	12	2	4	26.26	3.48	[5,17]
p03	Raw mill	12	2	4	8.48	1.13	[5,17]
p04	Preheater	25	15	5	6.78	0.64	[5,17]
p05	Precalciner	25	15	5	64.44	6.04	[5,17]
p06	Kiln	25	15	5	176.39	16.52	[5,17]
p07	Cooler	25	15	5	13.57	1.27	[5,17]
p09	Cement mill	12	2	4	15.00	1.99	[5,17]
p10	Finishing/Auxiliaries	12	2	4	28.34	3.76	[5,17]

Table 4
Technical characteristics of carbon capture options.

Production step		$Energy\ Required_{e,p,t}$ MJ/tonCO_2e		$CaptureRate_{i,p}$ & $CaptureRange_{i,p,pp}$		Sources
		e = electric	e = thermal			
p45	LEILAC	0		95%	Only precalciner	[38]
p48	Monoethanolamine (MEA)	887	3073	94%	All processes	[17]

Table 5
Design life and installation costs of carbon capture options.

Production step		$DesignLife_{p,f}$ (years)	Available (t)	$InstallationCost_{p,f,t}$ €/tonCO_2e		Sources
				Total	Annuity (f01/f02)	
p45	LEILAC	25	t20	100.00	9.34	[38]
p48	MEA	25	t05	76.00	7.12	[17]

Table 6
Energy Cost assumptions.

Energy source		$EmissionFuel_{s,i}$		$EnergyCost_{s,t}$	
		gCO_2/MJ	Sources	€/GJ	Sources
s01	Electricity	0		13.9	-
s02	Natural Gas	56.1	[41]	6.0	[17]
s03	Coal	81.1	[41]	3.0	[17]
s05	Hydrogen	0		27.1 (2020) /16.5 (2050)	[40] (long term)

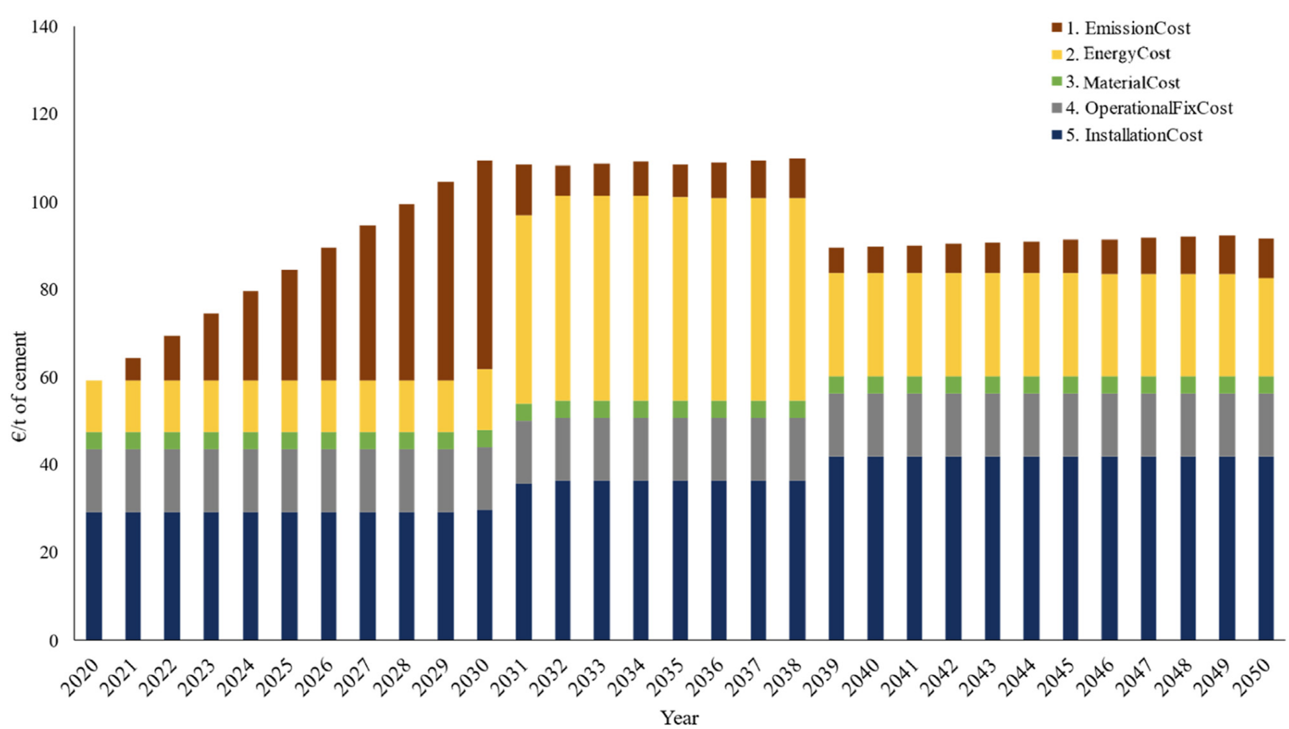

Fig. 1. Breakdown of relative costs of cement based on the operation of f01 and f02.

Table 7
Material cost assumptions [17].

Raw material		$MaterialCost_{i,t}$ (€/ton (i))
i01	Lime	1.6
i02	Sand	4.8
i03	Mineral additives	1.6
i11	Gypsum	3.2
i12	Mineral additions	6.4

Table 8
Process Emissions.

Production step		$EmissionProcess_{i,p}$ tCO_2/ ton (i)	Sources
p05	Precalciner	0.51	[17]
p06	Kiln	0.06	[17]
p45	LEILAC (precalciner)	0.51	[38]

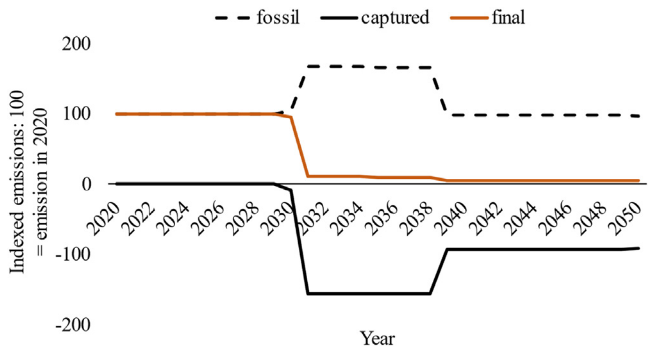

Fig. 2. Fossil emissions: captured and final atmospheric emissions.

As shown in Fig. 2, emissions from cement production decline only marginally until t09 = 2030 due to more efficient equipment installation. The energy requirements for the equipment are subject to an energy efficiency improvement factor for reinvestment at the end of its design life. The total fossil emission increase with the carbon capture technology because of the higher energy consumption of fossil fuels. However, emissions are captured, thus reducing atmospheric emissions to a minimum.

The LEILAC technology, installed at t20 = 2039, captures 95% of precalciner emissions, whereas the previously installed MEA technology captures emissions from the remaining processes, namely, the kiln. Because LEILAC requires less energy to operate, the total fossil and captured emissions decrease significantly after LEILAC is installed. As the model does not penalise equipment operation with only a fraction of its nameplate capacity, the parallel operation of the MEA and LEILAC appears logical. However, it remains unclear whether a parallel operation is feasible and whether modifications to the existing MEA technology are required to operate it jointly with LEILAC.

6. Discussion

The model results for the base case demonstrate the basic functionality of the model in one industrial sector and a single policy scenario, namely, the phase-out of free allowances for cement production combined with a continuously increasing CO_2 price. Thus, the model results do not allow for an in-depth comparison of industrial policies or potential effects when combining various industries and sector-specific policy options.

To realise the above, at least one additional sector, such as the steel industry, or (petro)chemical processes, such as fertiliser production, must be analysed. The modular formulation of the TRANSid model allows new sectors to be implemented by defining an additional material demand, such as the demand for steel, which must be satisfied and whose process steps *p* must be defined to produce it from raw materials in a new plant *f*.

Slight to no changes to the current model formulation are required to implement and analyse the different industrial policy options mentioned in the introduction. GPP can be modeled by introducing an additional demand for material type *i* that must comply with stricter emission limits in the early stage. Similarly, PCRs can be modeled by setting emission limits for all basic material demands. The EU ETS scenarios can be changed based on the CBAM by analysing different emission pricing scenarios and considering whether import and export flows should be considered (not yet implemented). The emission price in the current model design does not necessarily correspond to the EU ETS price but reflects the effective CO_2 price due to the free allowances currently granted to the industry. Similarly, CCfDs can be implemented in the model if installations of low-emission plants during the early phases of the transition are subject to alternative CO_2 price scenarios. The latter requires modifications to the current model design and the introduction of additional constraints to the model plant-specific CO_2 pricing.

The current model formulation and proposed additions allow a wide range of policy options to be analysed. Nevertheless, the model remains limited concerning emission, energy, and material market dynamics caused by different policy interventions as well as policies that require an understanding of macroeconomic dynamics, such as the evolution of a circular economy or cross-border trade. Elements of the proposed model can be used to extend, for example, energy system models that use material flows to reflect industrial transition and material circularity.

The proposed changes to the TRANSid model, particularly the extension to another sector, will increase the complexity of the optimisation problem. In the chemical industry, which involves highly integrated plant designs for processing hydrocarbons or renewable hydrogen and incorporating carbon-based feeds into different products, the high degree of technical complexity translates into increased mathematical complexity, rendering it difficult to obtain valid model results. Hence, the mathematical complexity of the model design must be reduced in the future, which may involve redesigning some parts of the formulation to obtain the optimal trade-offs for model depths, execution time, and result validity. Simultaneously, the model should be interoperable with energy system models such that interrelations between sector-specific policies and the energy and emission allowance markets can be investigated to provide coherent policy recommendations.

7. Conclusions

Understanding the effects of policy design options on the transformation of industries is key to a successful transition to emission-intensive basic material sectors. The TRANSid model allows one to understand the implications of different policy designs for one or several sectors. The presented case study in the cement sector demonstrates only the basic functionalities of the model. Nonetheless, the case study results provide some initial insights into the investment options. Carbon capture options in the cement sector are favoured, based on the fact that other alternatives do not reduce process emissions, indicating the willingness to retire emission-intensive processes prematurely if high CO_2 prices are expected. Furthermore, we used the results to outline how currently discussed policy options can be investigated using a more extensive case study involving several industries. Hence, in future studies, we plan to expand the TRANSid model to other sectors and perform a more comprehensive analysis of policies based on multiple technological, demand, and energy market price scenarios.

Declaration of competing interest

The authors declare that there are no conflicts of interest.

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