Implications of the EU ETS on the Level-Playing Field between Carbon Capture Storage & Utilisation

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Abstract

System modelling efforts have shown that carbon capture is a key technology to enable a cost-effective reduction of hard-to-abate emissions in energy-intensive industries. The CO_2 that is captured can either be utilised (CCU), or stored with carbon capture and storage (CCS). This paper examines the implications of both European carbon pricing mechanisms (ETS I & ETS II) on the level-playing field between CCS and CCU investments. Our contribution is threefold. First, we develop an equilibrium model that enables us to mimic market outcomes under different regulatory conditions. With a numerical case study applied to a fuel production chain, the model confirms that the current ETS regulation can have an adverse effect on CCU uptake. Especially with zero or low ETS II prices a lock-in effect can occur on CCS, potentially prolonging conventional refinery activities. Second, we propose an alternative approach to better integrate CCUS into the EU ETS. Results show that this approach maintains the level-playing field between CCU and CCS, regardless of any carbon price differentials. That results in a closer to Pareto optimal outcome in terms of welfare and emission abatement. Third, we present an analytic analysis to express the CCUS trade-off from a theoretical point of view. This provides generalised and concrete insights into how EU ETS influences the profitability and likelihood of CCUS. Our results help policymakers to gain a better understanding of the impact of ETS regulations on decarbonisation efforts in the industry.

Index Terms

Carbon Capture with Storage (CCS); Carbon Capture with Utilisation (CCU); Emission Trading System (ETS); Economic evaluation; Equilibrium modelling.

NOMENCLATURE

Sets (indices)

$\Omega_{\mathrm{T}}(t)$	Set of time steps (t = 1 year).

Variables

$\mathrm{q}_t^{\mathrm{CAP,\ CC_{DS}}}$	Invested capacity in downstream retrofitted carbon capture installation at time t [tonnes per annum (tpa)].
$\mathrm{q}_t^{\mathrm{CAP,\ CC_{US}}}$	Invested capacity in upstream retrofitted carbon capture installation at time t [tpa].

$q_t^{\text{CAP, CONV}_{\text{DS}}}$	Invested capacity in downstream conventional installation at time t [tpa].
$q_t^{\text{CAP, CONV}_{\text{US}}}$	Invested capacity in upstream conventional installation at time t [tpa].
$q_t^{\text{CAP, CU}_{\text{DS}}}$	Invested capacity in downstream carbon utilisation installation at time t [tpa].
$q_t^{\text{CU}_{\text{DS}}}$	Production quantity of downstream product by carbon utilisation at time t [tpa].
$q_t^{\text{CCS}_{\text{DS}}}$	Production quantity of downstream product by carbon capture installation send to storage at time t [tpa].
q_t^{CC}	Production quantity of upstream product by carbon capture installation at time t [tpa].
$q_t^{\text{CONV}_{\text{DS}}}$	Production quantity of downstream product by conventional process at time t [tpa].
$q_t^{\text{CCS}_{\text{US}}}$	Production quantity of upstream product by carbon capture installation send to storage at time t [tpa].
$q_t^{\text{CCU}_{\text{US}}}$	Production quantity of upstream product by carbon capture installation for re-use at time t [tpa].
$q_t^{\text{CONV}_{\text{US}}}$	Production quantity of upstream product by conventional process at time t [tpa].
$q_t^{\text{TOT, CC}_{\text{DS}}}$	Total installed carbon capture capacity downstream at time t [tp].
$q_t^{\text{TOT, CC}_{\text{US}}}$	Total installed carbon capture capacity upstream at time t [tp].
$q_t^{\text{TOT, CONV}_{\text{DS}}}$	Total installed conventional capacity downstream at time t [tp].
$q_t^{\text{TOT, CONV}_{\text{US}}}$	Total installed conventional capacity upstream at time t [tp].
$q_t^{\text{TOT, CU}_{\text{US}}}$	Total installed RFNBO capacity downstream at time t [tp].

Market prices

$\lambda_t^{\text{CO}_2}$	Trading price of the CO_2 commodity at time t [€/tCO_2].
p_t^{DS}	Price of the downstream product at time t [€/ton].
p_t^{US}	Price of the upstream product at time t [€/ton].

Parameters

$\alpha^{\text{CC}_{\text{DS}}}$	Downstream residual emission fraction after capture send to the atmosphere [-].
$\alpha^{\text{CC}_{\text{US}}}$	Upstream residual emission fraction after capture send to the atmosphere [-].
$\chi^{\text{CU}_{\text{DS}}}$	CO_2 emitted with CO_2 utilisation process to produce 1 ton of downstream product [tCO_2/ton].
$\chi^{\text{CONV}_{\text{DS}}}$	CO_2 emitted by the conventional process to produce 1 ton of downstream product [tCO_2/ton].
$\chi^{\text{CONV}_{\text{US}}}$	CO_2 emitted by the conventional process to produce 1 ton of upstream product [tCO_2/ton].
$\Phi^{\text{CU}_{\text{DS}}}$	Amount of tonnes CO_2 required to produce 1 ton of downstream product [tCO_2/ton].
$\Phi^{\text{USE}_{\text{DS}}}$	Amount of tonnes CO_2 emitted after usage downstream [tCO_2/ton].
τ	Discount rate [-].
A^{DS}	Intercept of demand curve for downstream product [€/ton].
A^{US}	Intercept of demand curve for upstream product [€/ton].
B^{DS}	Slope of demand curve for downstream product [€/ton^2].
B^{US}	Slope of demand curve for upstream product [€/ton^2].
$C^{\text{CAP, CC}_{\text{DS}}}$	CAPEX of carbon capture installation for downstream industry per ton CO_2 captured [€/tCO_2].
$C^{\text{CAP, CC}_{\text{US}}}$	CAPEX of carbon capture installation for upstream industry per ton CO_2 captured [€/tCO_2].
$C^{\text{CAP, CONV}_{\text{DS}}}$	CAPEX of conventional installation for downstream industry per ton production [€/ton].

$C^{\text{CAP, CONV}_{\text{US}}}$ CAPEX of conventional installation for upstream industry per ton production [€/ton].

$C^{\text{CAP, CU}_{\text{DS}}}$ CAPEX of carbon utilisation installation for downstream industry per ton CO_2 utilised [€/tCO_2].

$C_t^{\text{ETS II}}$ Cost of European emission allowance under ETS II at time t [€/tCO_2].

$C_t^{\text{ETS I}}$ Cost of European emission allowance under ETS I at time t [€/tCO_2].

C_t^{E} Cost of electricity at time t [€/kWh].

$C_t^{\text{fuel}_{\text{DS}}}$ Cost of fossil fuel for downstream industry [€/kWh].

$C_t^{\text{fuel}_{\text{US}}}$ Cost of fossil fuel for upstream industry [€/kWh].

C^{S} Cost of CO_2 storage [€/tCO_2].

C^{T} Cost of CO_2 transport [€/tCO_2].

$E^{\text{CC}_{\text{DS}}}$ Electricity consumption to capture 1 ton of CO_2 by downstream industry [kWh/tCO_2].

$E^{\text{CC}_{\text{US}}}$ Electricity consumption to capture 1 ton of CO_2 by upstream industry [kWh/tCO_2].

$E^{\text{CONV}_{\text{DS}}}$ Fossil fuel consumption to produce 1 ton of downstream product with conventional installation [kWh/ton].

$E^{\text{CONV}_{\text{US}}}$ Fossil fuel consumption to produce 1 ton of upstream product with conventional installation [kWh/ton].

$E^{\text{CU}_{\text{DS}}}$ Electricity consumption to purify and process 1 ton of CO_2 to convert it into downstream product (incl. electricity for hydrogen production) [kWh/tCO_2].

$Q_{t=0}^{\text{CONV}_{\text{DS}}}$ Initial installed conventional capacity of downstream industry [ton].

$Q_{t=0}^{\text{CONV}_{\text{US}}}$ Initial installed conventional capacity of upstream industry [ton].

T^{OPT} Optimisation period [years].

T^{DS} Lifetime downstream production facility [yrs].

T^{US} Lifetime upstream production facility [yrs].

Case parameters

$\mathcal{Z}^{\text{ETS}^*_{I,\text{DS}}}$ Binary parameter, 1= downstream carbon utilisation industry falls under ETS I regulation [-].

$\mathcal{Z}^{\text{ETS}_{I,\text{DS}}}$ Binary parameter, 1= downstream fossil-based industry falls under ETS I regulation [-].

$\mathcal{Z}^{\text{ETS}^*_{I,\text{US}}}$ Binary parameter, 1= upstream industry falls under ETS I regulation, but needs to surrender all captured emissions [-].

$\mathcal{Z}^{\text{ETS}_{I,\text{US}}}$ Binary parameter, 1= upstream industry falls under ETS I regulation [-].

$\mathcal{Z}^{\text{ETS}^*_{II,\text{DS}}}$ Binary parameter, 1= downstream industry falls under ETS II regulation, synthetic (indirect fossil fuels) are covered [-].

$\mathcal{Z}^{\text{ETS}_{II,\text{DS}}}$ Binary parameter, 1= downstream industry falls under ETS II regulation, fossil-based fuels are covered [-].

The parameter values used can be found in Appendix A.

1. Introduction

Amidst the urgency of addressing climate challenges, there is a crucial need for substantial global decarbonisation efforts. Particularly the industrial sector, which accounts for approximately 30% of global emissions, has encountered difficulties in implementing low-carbon solutions [1]. To overcome these challenges, the adoption of Carbon Capture Utilisation & Storage (CCUS) is anticipated to play a vital role in achieving rapid and significant emission reductions within the industry [1, 2].

The capture of CO_2 emitted by industrial and power sectors remains relatively low on a global scale. Roughly 0.1% of global CO_2 emissions, or 25 to 45 million tonnes (Mton) of CO_2 is being captured annually [3, 4]. The International Energy Agency indicates, however, that these current capturing levels should drastically upscale to more than 6000 Mton per year by 2050 to comply with the net-zero ambition. From that amount, 50% up to 95% is expected to be stored geologically which leaves the remainder to be devoted to utilisation purposes such as e-fuel production [5, 6].[1]

The adoption of CCUS technologies in relation to the emission reduction targets in Europe will require appropriate policies that incentivise investments thereof. This should ideally be accomplished by pricing carbon emissions such that marginal damages are internalised. In the EU, the Emission Trading System (ETS) has been covering emissions from the power sector and energy-intensive industries for nearly two decades. A second ETS will furthermore be operational from 2027 onward and targets emissions from fuel consumption in buildings and road transport. Throughout this paper, we will refer to the former as ETS I and the latter as ETS II.

This paper investigates the impact of both ETS systems (EU ETS I & II) on CCS and CCU adoption. We argue that the EU ETS regulation could distort the CCS and CCU investments if EU ETS II price levels are not harmonised with EU ETS I prices. Lower ETS II prices might lock in too much CCS compared to what would be desired from a welfare and emission abatement perspective. We therefore additionally propose an alternative ETS configuration that is more robust against carbon price differentials. Modelling efforts confirm that the current ETS framework indeed may be subject to such investment distortions and that this new proposal maintains an equilibrium that is closer to the optimum.

The remainder of this paper is structured as follows. In Section 2, we first provide a survey of the emission abatement potential of CCU and CCS, followed by the governing EU ETS regulation, as well as an overview of the related literature in relation to the contribution of this paper. Section 3 presents the modelling framework and introduces the numeric case study applied to the different regulatory cases. The analysis can be found in the result section, Section 4, which assesses the effect of ETS (I & II) pricing regulations on (i) the investment trade-off between CCS & CCU, (ii) the resulting CO_2 commodity trading price if CCU takes place, and (iii) welfare and emission implications of the ETS regulation. This is done by providing both a numeric and analytic analysis. Section 5 concludes this work. Note that the term ‘CO_2 commodity trading price’ denotes the price of CO_2 used as a feedstock for the production of e-fuels or chemicals downstream the value chain and should not be confused with the price of carbon emission allowances (ETS I or II prices).

2. Literature & context

2.1 Emission abatement potential in view of CCUS

In what follows, we aim to conceptually explain the differences in emissions abated by CCS and CCU. These insights will be leveraged later when discussing how policies should be designed to abate emissions efficiently. Both production routes are illustrated in 1, in which the top window indicates the conventional production route with CCS, while the CCU route that

[1] E-fuels can be produced combining (green) hydrogen and captured CO_2 in processes like Fischer-Tropsch synthesis, methanol synthesis or methanation.

utilises CO_2 is depicted in the bottom window. This illustration comprises an upstream firm that captures its emitted CO_2 at an emission point source and a downstream firm that potentially reuses this captured CO_2 to produce fuels. Note that in both of the production routes unavoidable end-use emissions occur due to the use or combustion of fuels by downstream users.[2]

In the case of conventional production with CCS, the downstream fuel production process resorts to oil extraction and mineral oil refining with carbon capture, as can be seen in the top window of 1. A large fossil dependency remains and residual emissions originate from (i) fossil fuel end-use and (ii) capture inefficiencies both upstream and downstream. A carbon-neutral scenario would consequently require additional direct air capture (DAC) or bio-energy carbon capturing (BECC) with storage. Carbon capture, in general, should hence be predominantly adopted in industries with hard-to-abate emissions like unavoidable process emissions or high-temperature heat requirements such as in cement, iron & steel and chemical production facilities [3]. In other cases, renewable-based, carbon-free alternatives like the use of hydrogen and electrification could be better suited.

Some sectors like the aviation, shipping and chemical sectors are projected to remain dependent on carbon-based feedstock or fuels [5]. CCU could contribute here by creating synergies between hard-to-abate upstream industries and downstream carbon-based fuel producers, as depicted in the bottom window of 1. The reuse of carbon is accompanied by a new type of downstream installation that is capable of producing e-fuels derived from CO_2 and hydrogen (H_2). To make sure that these e-fuels are created from sufficiently low-carbon energy, the EU has introduced a new label for these fuels: Renewable Fuels of Non-Biologic Origin (RFNBOs),[3] together with some quota[4] expressing the share of RFNBOs in the European fuel mix [7, 8]. The simplest form of RFNBO is green hydrogen, but also complex hydrocarbon fuels like e-kerosene can be considered RFNBO.

To qualify as an RFNBO product, greenhouse gas (GHG) emissions should be reduced by at least 70% compared to the fossil equivalent. It depends on the timeframe whether or not CO_2 captured from fossil-derived sources is eligible for this criterion. Indeed, a distinction can be made between two stages, depicted by (1) and (2) in 1. During the first stage, CO_2 captured from fossil sources upstream will be considered avoided in the downstream product. In that way, the 70% reduction threshold can be obtained allowing to qualify the downstream fuel as an RFNBO product [8, 9]. Nevertheless, as the CO_2 contained in the RFNBO product still has a fossil origin, combustion of the fuel will keep adding emissions to the atmosphere. To avoid the continuous use of fossil fuels upstream and the related additional fossil-related end-use emissions, the regulation qualifying for RFNBOs that applies to (1) intends to only hold up to 2035 for electricity generation with capture and up to 2040 for other industry-related capturing processes [10]. Afterwards, RFNBOs are mainly to be produced with atmospheric or biogenic CO_2 using DAC or BECC technologies, depicted by (2) in 1. In that way, the use of fossil CO_2 and any related additional emissions are avoided as biogenic or atmospheric CO_2 keeps circulating. Hence, carbon loops can be closed. Combined with zero-emission energy for capture and conversion processes, this pathway allows to minimise the fossil and storage dependency while being Paris compatible[5] [12].

[2]Products other than fuels also cause emissions, but these are often not related to the product-use phase, but more to the disposal phase. Here, waste incinerators or recycling plants could be retrofitted with carbon capture which allows to avoid most of the emissions escaping to the air.

[3]Note that the ‘non-biological origin’ refers to the origin of the energy provided to make RFNBOs and not to the origin of the CO_2 contained in the fuel. This CO_2 could come from biomass as well.

[4]Current quotas, expressed by the RED III directive, indicate a minimum of 1% share of RFNBOs in the transport sector and 42% in the industry by 2030 [7].

[5]Referring to the Paris Agreement as signed in 2015 by all world’s nations to pursue efforts keeping global temperatures below 1.5 °C of pre-industrial levels [11].

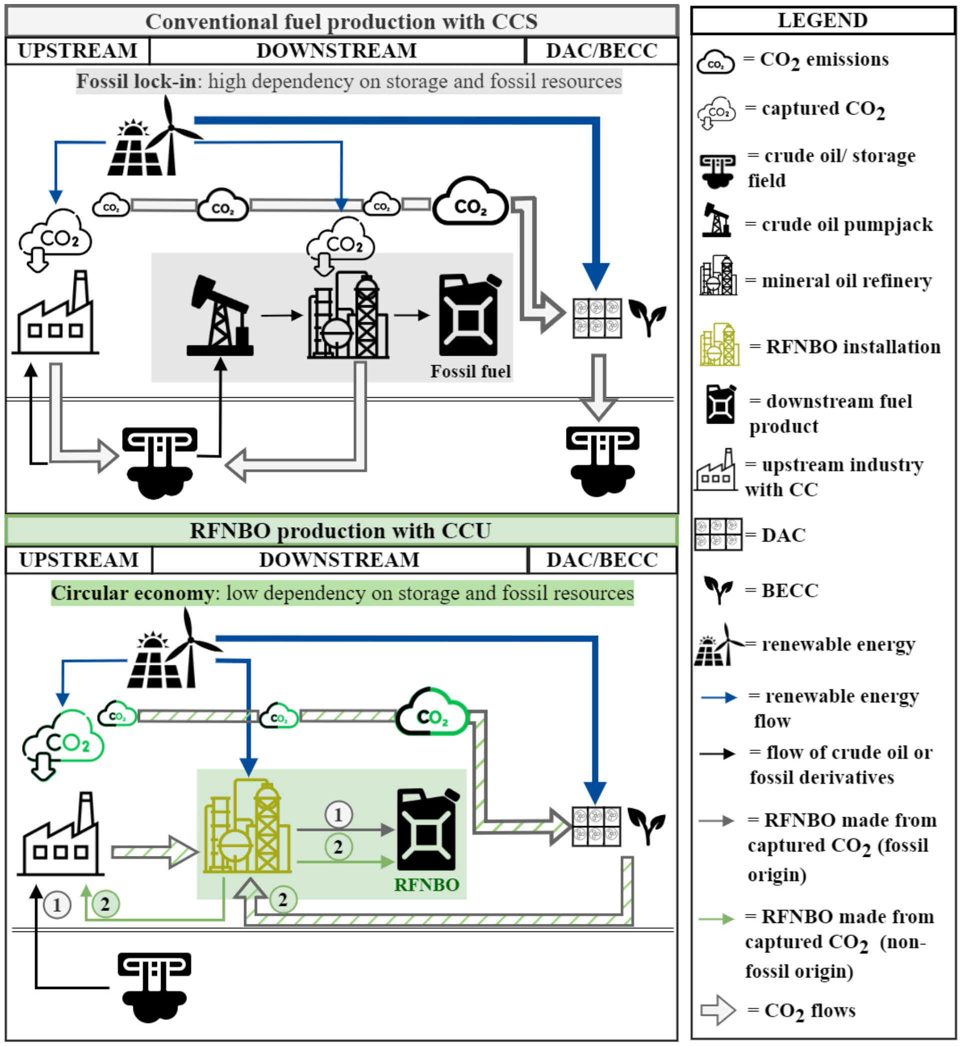


Fig. 1: Two different fuel production routes resulting in the same end-product (fuel) and net zero emissions. The top route is largely dependent on fossil resources, CO_2 storage and requires negative emission technologies with storage (DACS, BECCS). The bottom route creates a circular economy with less storage and fossil resource dependency by utilising captured CO_2 from fossil, biogenic (BECC) or atmospheric (DAC) origin (source: authors).

To summarise 1, CCS can serve its potential in hard-to-abate industries. However, a transformation of refineries to RFNBO production facilities will be needed to reach the net-zero target without major fossil lock-ins. To boost this transition, adequate levels of captured CO_2 should be available, ideally from biogenic or atmospheric origin. Nonetheless, studies have shown that it might be necessary to compensate for insufficient supply projections of biogenic or DAC-derived CO_2 for the production of fuels and chemicals [13]. Therefore, promoting CCU processes that capture fossil-derived CO_2 from industry point sources could enable a faster and smoother transition [12, 14]. Although the European regulation does recognise this in the context of the 70% RFNBO qualification target, we do foresee potential issues in the EU ETS regulation as will be explained next.

2.2 *Emission abatement policies in view of CCUS: EU ETS I & II*

2.2.1 *EU ETS I:*

Most of the jurisdictions related to CCUS in combination with the EU ETS I[6] are contained in the EU Directive 2003/87/EC [15]

[6]EU ETS I here refers to the EU ETS system that came into force in 2005, not to be confused with ETS II as announced in 2022.

accompanied by its monitoring and reporting guidelines [16]. Articles 48 and 49 of the latter document are of particular interest to us. Article 48 dictates that CO_2 captured and transferred to an installation should be included in the emission factor of the source stream. Phrased differently, an upstream installation needs to surrender carbon allowances for its captured and transferred emissions. This has been included to avoid emission leakage out of the ETS I when carbon dioxide is transferred to non-ETS I installations[7]. There are two notable exceptions to this rule. First, the upstream firm is exempt from surrendering allowances if both installations are covered by the EU ETS system, in which case the downstream firm will surrender allowances when emitting the CO_2. Second, the upstream firm does not need to surrender allowances when CO_2 is used for geological storage or permanently chemically bound in precipitated calcium carbonate (PCC) as defined in Article 49 [17]. This can be motivated by the time at which carbon is released into the atmosphere. Generally speaking, carbon is priced unless 'permanently' bound.

The current ETS regulation hence provides an incentive for CCS since upstream firms do not need to surrender allowances when permanently storing carbon. On the other hand, the regulation does not provide an incentive to capture and transfer CO_2 to non-ETS I sectors, like RFNBO production facilities, for utilisation. Upstream firms will, in that case, need to surrender allowances as if they had emitted the carbon into the atmosphere themselves. Capturing and transferring carbon to non-ETS sectors can still transpire if economically interesting, i.e. if signalled via carbon commodity prices that are sufficiently high to also cover the ETS I allowance cost. Nonetheless, the ETS I design favours CCS above CCU if the carbon is being utilised by non-ETS sectors. This can be efficient because an allowance is surrendered for each unit of carbon that ends up in the atmosphere, regardless of whether it is emitted directly or indirectly via the CCU route. Crucially, however, this line of argument does not necessarily hold if conventional, fossil fuels are not covered evenly by ETS credits or taxes. Here, the interaction with ETS II becomes important, which we turn to next.

2.2.2 EU ETS II:

A second emission trading system, ETS II, has been announced to increase the fraction of emissions covered by carbon pricing mechanisms and will take effect from 2027 onward. It will be implemented in parallel to ETS I and covers fuel use in commercial and residential buildings and road transportation[8], as well as the use of fuels in manufacturing and construction industries. The ETS II mechanism would function similarly to the current ETS mechanism and although it is difficult to make any claims on the expected ETS II price, the EU institutions have taken measures to keep it below 45 €/tCO_2 as far as possible, at least until 2030 [18, 19].

The EU ETS II system should comply with the EU vision, that: *'all emissions are accounted for and that double counting is avoided while generating economic incentives'* [20]. Double counting in this context occurs when for instance an RFNBO made from fossil upstream CO_2 is covered twice by the EU ETSs: once by upstream surrendering of EU ETS I credits for the transferred CO_2, and once by ETS II for the same CO_2 now contained in a product and emitted during the product-use phase. For that reason, RFNBO-qualified products are not supposed to be covered by EU ETS II, thereby avoiding double counting.

[7] A common example is the ammonia industry covered by the ETS that needs to surrender carbon credits for all CO_2 that is transferred to a urea production facility not being covered by the ETS [17].

[8] Excluding agricultural vehicles on paved roads.

2.2.3 EU ETS I & II combined:

The main issue arises when the EU ETS I price differs from the EU ETS II price. As mentioned, the EU institutions aim to keep the ETS II price below 45 €/tCO_2, which is roughly half of today's ETS I price. The use of RFNBOs derived from upstream non-bio-based CO_2 relative to the use of fossil fuels gets disfavoured economically. A toy example in Fig. 2 has been created to better understand this distortion.

Similarly as in Fig. 1, an upstream and downstream industry is represented where the downstream industry either decides to continue producing fossil fuels (left) or changes to RFNBO production using CO_2 from an upstream industrial carbon capture plant (right). The numbers indicate the flow of carbon that is contained in a fuel or has been emitted or stored. The cells underneath indicate for each option and each case how the ETSs cover the different CO_2 fractions.

Under 'Case 1', the explained ETS regulation is presented combining the current ETS I system with the projected ETS II regulation. Although the same amount of emissions is covered for both production options, part of the emissions belong to different ETS systems. A low ETS II price ($C^{\text{ETS II}}$) compared to ETS I ($C^{\text{ETS I}}$) will bias the equilibrium towards the conventional production route with CCS as the latter will require less allowance spending than the CCU route.[9] A lower ETS II price, or the absence of an ETS II system altogether, hence artificially increases the production competitiveness of fossil fuels and decreases the willingness to pay for the CO_2 commodity by downstream firms. Lower carbon commodity prices, in turn, favour carbon storage over carbon utilisation. The industrial decarbonisation route could therefore lock in too much carbon storage relative to carbon utilisation. Only under equal price levels, no distortion take place and the cost for the 80 ETS I credits upstream will be internalised by the carbon commodity price. Vice versa, if the ETS II price would exceed the ETS I price, CCS would be economically disfavored against CCU.

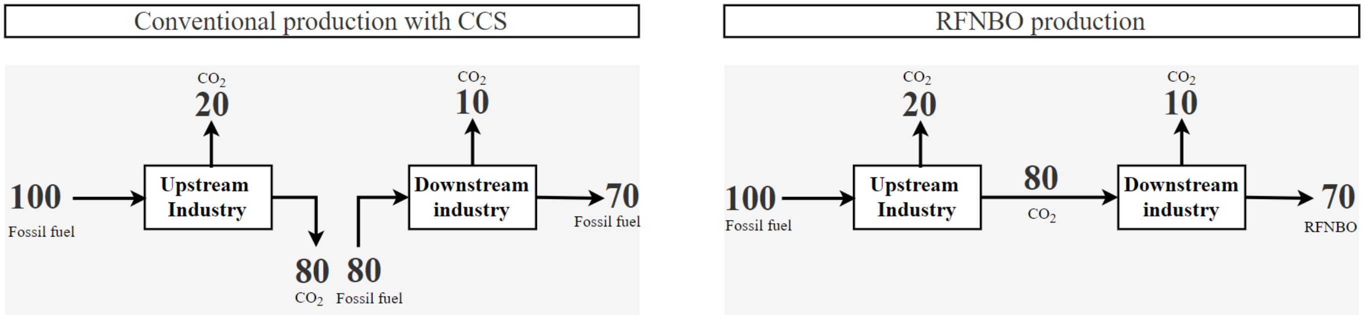
An alternative ETS configuration is proposed in this study indicated by 'Case 2'. Surrendering of ETS I credits on traded CO_2 feedstock is now replaced by ETS II credits on the downstream emissions related to fuel usage. We argue that this proposed case is more consistent by providing the same ETS coverage for both production routes in contrast to Case 1. Regardless of the production route, even with different ETS price levels, the allowance spending is identical. Case 2 would hence not distort the trade-off between the CCU and CCS production route.

2.3 Related literature & paper contribution

So far, we have qualitatively identified that CCU might be economically disfavored relative to CCS with the current ETS system. Other policy-driven studies have reached similar conclusions regarding ETS I [8, 21, 22]. Nevertheless, these studies do not touch upon the potential CCS lock-in effect nor discuss the ETS II impact. A more model-oriented approach, as aimed for in this paper, should give a more profound understanding of the combined EU ETS effect on the level-playing field between CCS (or conventional fuel production) and CCU.

Several modelling-driven studies in the literature performed techno-economic analyses for dedicated industries assessing the effects of the ETS regulation. Onarheim et al. adopted six different scenarios with different carbon pricing regulations to calculate the levelised cost of pulp and board. The authors conclude that under the current EU ETS BECC is not stimulated

[9]The CCS route would require $30 \cdot C^{\text{ETS I}} + 70 \cdot C^{\text{ETS II}}$, whereas the CCU route would require $100 \cdot C^{\text{ETS I}}$. The former is clearly more attractive if the ETS II allowance price is lower than the ETS I allowance price.



	Upstream	Downstream
Case 1	(20) . $C^{ETS\ I}$	(10) . $C^{ETS\ I}$ + **(70)** . $C^{ETS\ II}$
Case 2	(20) . $C^{ETS\ I}$	(10) . $C^{ETS\ I}$ + (70) . $C^{ETS\ II}$

	Upstream	Downstream
Case 1	(20 + **80**) . $C^{ETS\ I}$	0
Case 2	(20) . $C^{ETS\ I}$	(10) . $C^{ETS\ I}$ + (70) . $C^{ETS\ II}$

Fig. 2: Simplified example stressing the distortion of the ETS regulation on CCU and CCS under the two different policy cases. Case 1 represents the governing ETS I & II regulation for which ETS I allowances need to be surrendered when CO_2 is traded to the RFNBO installation. Case 2 represents the proposed ETS configuration. Here, all fuels with fossil CO_2 are covered by ETS II, no upstream surrendering of traded CO_2 takes place.

when no revenue stream is obtained for the captured negative CO_2 emissions coming from pulp production. This financial incentive could potentially come from carbon offsets (BECCS credits) or by selling their biogenic captured CO_2 to RFNBO producers, something that was not addressed in their study [23]. In contrast, Strunge et al. do consider the reutilising potential of CO_2. This has been investigated for the production of supplementary cementitious materials (SCM) in the cement industry. In their pessimistic scenario, the CO_2 used in SCM has not been exempted from EU ETS allowance surrendering which significantly reduces the profits per tonne of SCM produced. Furthermore, the authors compare the SCM-utilisation pathway as well with other CCU and CCS-related production routes for cement-derived CO_2 under different EU ETS price levels. They conclude that combining two production routes: oxyfuel CCS with CO_2 mineralisation might result in the lowest levelised cost of cement [24]. The reuse of CO_2 could also take place beyond one industry. In that regard, Yao et al. addressed different business models for CO_2 trading ranging from vertical integration to more market-driven designs [25]. Such market-driven designs could especially be promising in regions with high re-utilisation potentials such as the industrialised regions in Belgium (Antwerp, East Flanders) and Germany (Dusseldorf and Cologne) as stated by Butnar et al. [6]. The market-based approach in which two separate (non-integrated) entities trade CO_2 has been included in other modelling studies as well [26, 27]. Here, Cabrera et al. used a more stylised modelling approach to assess the effect of carbon pricing on technological investment decisions. With an equilibrium model formulation, the authors investigate the effect of a carbon tax on CCU and CCS investment with the goal of evaluating the resulting emissions [26]. From their analysis, it becomes clear that climate policies could have an adverse effect on emission outcomes depending on certain market dynamics.

Our contribution is threefold. First, to the best of the authors' knowledge, this study is the first to unveil that the foreseen EU ETS distorts the level playing field between CCU and CCS. This could discourage carbon-based e-fuel production, likely prolonging conventional refinery processes through the upstream surrendering of carbon credits and potential differences in ETS I & II price levels. In that regard, we develop an equilibrium model to examine the magnitude of these effects in terms of CCUS-related investments, abated emissions and welfare implications. Our model extends the work of Cabrera et al. [26]

by considering a multi-year time horizon and by including the ETS aspects. Second, we propose and analyse an alternative configuration of ETS I & II that intends to restore the level-playing field between CCU and CCS and is more robust with respect to ETS price differentials. Third, a theoretical analysis is provided that allows us to express the conditions under which e-fuel production takes place. This analysis analytically conceptualises the trade-off between the CCU technology pathways and other production routes, considering the different ETS cases. It allows us to explain modelling outcomes and provides more intuition concerning result sensitivities. We apply the analysis to one particular case study (upstream steel producer and downstream fuel producer) to show the practical applicability of the analytic framework. It can be conveniently extended to other case studies as well.

3. Model & Case Study

3.1 Model set-up

The results of this study are generated with an equilibrium model that is used to express the investment and operational decisions of each of the involved market participants over a multi-year horizon. Although we present and interpret our model as an equilibrium model, it can be efficiently solved by recasting it as an equivalent single-objective optimisation model[10] since it satisfies the conditions listed in [28]. The equivalent optimisation model has been implemented using the JuMP (Julia for Mathematical Optimization) library [29] and solved with the Gurobi Solver [30].

Fig. 3 schematises the modelling framework. The white boxes indicate four different market participants: an upstream industry, a downstream industry, upstream consumers of the upstream product and downstream consumers of the downstream product. Upstream and downstream products are sold to their respective consumers via the product markets, represented by the grey (solid) boxes. Consumers are price-responsive i.e. the framework allows to capture changes in product demand due to changes in prices. Product prices, in turn, are endogenous and can vary with the policy situation. The symbols next to the arrows correspond to quantities and prices, which can be interpreted together with the model equations.

Upstream an industrial production process is represented. As indicated by the top-left box in Fig. 3, this upstream product can be produced using three different routes: conventionally, with retrofitted carbon capture in which CO_2 is stored (CCS), or with retrofitted carbon capture while CO_2 is traded for utilisation purposes (CCU).

When the upstream industry decides to capture and trade CO_2 instead of storing it, it can be traded in the CO_2 commodity market to the downstream producer. This downstream producer is considered to be a fuel producer that again has three production options. Two of the options relate to fuel production with mineral oil refining in which CO_2 is emitted or partly captured and stored. These are the conventional and CCS production routes respectively. The third production strategy occurs when the downstream industry decides to invest in a completely new production installation for the production of RFNBOs by reusing CO_2 from the upstream industry. In that way, they participate in the CO_2 commodity trading market. Note that the CO_2 commodity price ($\lambda_t^{\mathrm{CO}_2^*}$) is endogenously determined by the model. The resulting downstream product will no longer be indicated as 'fossil fuel', but it gets the term 'RFNBO' assuming that the energy used for production is sufficiently green. We

[10]Of which the objective is presented in Appendix B.

abbreviate this downstream route as CU, carbon utilisation. Combined with the carbon capture and utilisation route upstream, the abbreviation C(C)U is used.

The model assumes a fully deterministic setting with perfectly competitive and rational agents. We consider just one type of upstream and downstream industry and CO_2 cannot be reused within the same industry. Investment decisions of those industries have an immediate effect on production capacities to simplify the model formulation, i.e. no lead time is considered. Finally, the EU ETS systems are exogenously integrated into the model as carbon taxes whether or not with the same price levels.

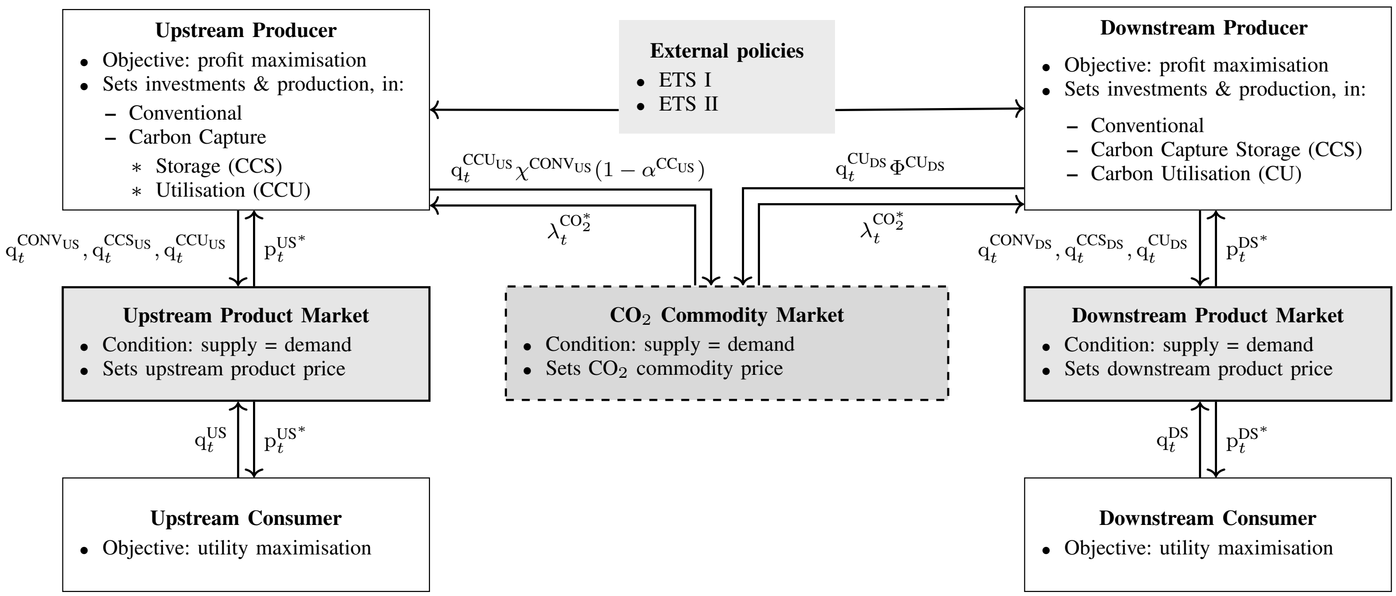


Fig. 3: Illustration of the model framework with 4 market players (white boxes) and 3 markets (grey boxes). Each producer has 3 production decisions. When C(C)U is chosen, CO_2 is traded over a CO_2 commodity market.

The objectives with related constraints of each market participant schematised by Fig. 3 are given below. The equilibrium formulation allows for identifying trading in three different markets: the upstream product, the downstream product and potentially the CO_2 commodity market. Producers optimise capacities and production quantities taking prices as given. Consumers do the same in relation to the amounts of product consumed. The symbols and their interpretation are presented in the nomenclature. The equations hold for each year $t \in \Omega_T$ unless otherwise specified.

3.1.1 Upstream industry:

The upstream industry has the objective to maximise its discounted profits Π_t^{US} for the optimisation period as in Eq. (1), expressed as the obtained revenues $\mathcal{R}_t^{US}$ minus the incurred costs $\mathcal{C}_t^{US}$. The revenues and costs are covered by expression (2)-(5). The CO_2 commodity trading price ($\lambda_t^{CO_2{}^*}$) in (2) is expressed as revenue to the upstream industry, meaning that a positive price in (2) will imply revenues for the upstream side. Logically, selling upstream products at a certain price ($p_t^{US^*}$) is also regarded as revenue to the upstream producers. The upstream product can be obtained from three different production routes i.e. conventional production ($q_t^{CONV_{US}}$) or conventional production retrofitted with carbon capture leading to CCS ($q_t^{CCS_{US}}$) or

CCU ($q_t^{CCU_{US}}$).

The costs are expressed as the sum of the capital costs and the operational costs by Eq. (4) and (5) respectively. The capital costs contain the sum of the capital expenditures for retrofitted carbon capture and for building higher capacities of conventional installations. As the capital expenditures for carbon capture $C^{CAP,\,CC_{US}}$ are expressed in €/tCO$_2$, the capacity of captured production quantity ($q_t^{CAP,CC_{US}}$) is multiplied with the amount of CO_2 captured per tonne of product $\chi^{CONV_{US}}(1-\alpha^{CC_{US}})$. In this term, $\chi^{CONV_{US}}$ stands for the released carbon per tonne of product and $(1-\alpha^{CC_{US}})$ the capture efficiency. To account for the remaining salvage value of assets at the end of the optimisation period a depreciation factor is applied to the capital expenditures. As such, an investment made at the end of the optimisation period with $t = T^{OPT}$ will have a high remaining salvage value, such that only one year of the asset lifetime is accounted for in the CAPEX balance.

The operational expenditures comprise the fuel cost of production, the energy (heat and electricity) costs for capturing carbon, the storage and transport costs for CO_2 removal and the costs related to the ETS policy. The latter is composed of ETS credits for (residual) emissions released into the atmosphere and ETS credits for transferring CO_2 emissions to the downstream industry. The binary parameters $\mathcal{Z}^{ETS...}$ allow to activate or deactivate these ETS terms to model different regulatory case studies. Tab. II in Appendix A links the value of the binary parameters ($\mathcal{Z}^{ETS...}$) to the considered case. In the case CO_2 is sold to a downstream industry, the transportation costs are assumed to be shared equally between the seller and buyer.[11]

$$\max_{q_t^{US}} \sum_{t\in\Omega_{T^{OPT}}} \Pi_t^{US} = \sum_{t\in\Omega_{T^{OPT}}} \frac{1}{(1+\tau)^t}(\mathcal{R}_t^{US} - \mathcal{C}_t^{US}) \tag{1}$$

$$\mathcal{R}_t^{US} = \overbrace{p_t^{US^*}(q_t^{CONV} + q_t^{CCS} + q_t^{CCU})}^{\text{Revenues from upstream product}} + \overbrace{\boldsymbol{\lambda_t^{CO_2 *}} q_t^{CCU_{US}} \chi^{CONV_{US}}(1-\alpha^{CC_{US}})}^{\text{Revenues from } CO_2 \text{ commodity trading}} \tag{2}$$

$$\mathcal{C}_t^{US} = \mathrm{CAPEX}_t^{US} + \mathrm{OPEX}_t^{US} \tag{3}$$

$$\mathrm{CAPEX}_t^{US} = \overbrace{\frac{T^{OPT} - t + 1}{T^{US}}}^{\text{Depreciation term}} \left(\overbrace{C^{CAP,\,CC_{US}} q_t^{CAP,CC_{US}} \chi^{CONV_{US}}(1-\alpha^{CC_{US}})}^{\text{CAPEX or retrofit carbon capture unit}} + \overbrace{C^{CAP,\,CONV_{US}} q_t^{CAP,\,CONV_{US}}}^{\text{CAPEX conventional unit}} \right) \tag{4}$$

[11]Note that some costs, like operation and maintenance costs, are disregarded, likewise, non-energy or carbon-related feedstock as these are assumed to be the same between the technology pathways, only adding more complexity to the model representation.

$$\begin{aligned}\mathrm{OPEX}_t^{\mathrm{US}} = \; & \overbrace{\mathrm{q}_t^{\mathrm{US}} \mathrm{E}^{\mathrm{CONV_{US}}} \mathrm{C}_t^{\mathrm{fuel_{US}}}}^{\text{Fuel costs for conventional product and product with capture}} \quad + \overbrace{\mathrm{q}_t^{\mathrm{CC_{US}}} \mathrm{E}^{\mathrm{CC_{US}}} \chi^{\mathrm{CONV_{US}}} (1-\alpha^{\mathrm{CC_{US}}}) \mathrm{C}_t^{\mathrm{E}}}^{\text{Electricity cost for product with capture}} \\ & + \overbrace{\mathrm{q}_t^{\mathrm{CCS_{US}}} \chi^{\mathrm{CONV_{US}}} (1-\alpha^{\mathrm{CC_{US}}})(\mathrm{C}^{\mathrm{T}} + \mathrm{C}^{\mathrm{S}})}^{\text{Transport \& storage costs for product with capture to storage}} + \overbrace{\mathrm{q}_t^{\mathrm{CCU_{US}}} \chi^{\mathrm{CONV_{US}}} (1-\alpha^{\mathrm{CC_{US}}})(\mathrm{C}^{\mathrm{T}}/2)}^{\text{Transport costs for product with capture to RFNBO}} \\ & + \overbrace{\mathcal{Z}^{\mathrm{ETS}_I,\mathrm{US}} (\mathrm{q}_t^{\mathrm{CC_{US}}} \alpha^{\mathrm{CC_{US}}} \chi^{\mathrm{CONV_{US}}} + \mathrm{q}_t^{\mathrm{CONV_{US}}} \chi^{\mathrm{CONV_{US}}}) \mathrm{C}_t^{\mathrm{ETS}_I}}^{\text{ETS I costs for (residual) emissions from conventional product and product with capture}} + \overbrace{\mathcal{Z}^{\mathrm{ETS}^*_I,\mathrm{US}} \mathrm{q}_t^{\mathrm{CCU_{US}}} \chi^{\mathrm{CONV_{US}}} (1-\alpha^{\mathrm{CC_{US}}}) \mathrm{C}_t^{\mathrm{ETS}_I}}^{\text{ETS I costs for transferred } \mathrm{CO_2} \text{ emissions}} \end{aligned} \tag{5}$$

Eq. (6) defines the production with carbon capture as the sum of production with CCS and CCU so that carbon is either stored or sent to a downstream utilisation facility. The total installed conventional capacity and total carbon capture capacities are tracked over time by Eq. (7) and (8). For Eq. (7) legacy capacity can be considered at time t equal to zero. These equations take into consideration the retrofitting of conventional installation by carbon capture units. Finally, Eq. (10) ensures that production with a certain technology does not exceed the total installed capacity available that year.

$$\mathrm{q}_t^{\mathrm{CC_{US}}} = \mathrm{q}_t^{\mathrm{CCS_{US}}} + \mathrm{q}_t^{\mathrm{CCU_{US}}} \tag{6}$$

$$\mathrm{q}_t^{\text{TOT, CONV}_{\mathrm{US}}} = \begin{cases} \mathrm{Q}_{t=0}^{\mathrm{CONV_{US}}}; \quad t=0 \\ \mathrm{q}_{t-1}^{\text{TOT, CONV}_{\mathrm{US}}} + \mathrm{q}_t^{\text{CAP, CONV}_{\mathrm{US}}} - \mathrm{q}_t^{\text{CAP, CC}_{\mathrm{US}}}; \quad \forall t \neq 0 \end{cases} \tag{7}$$

$$\mathrm{q}_t^{\text{TOT, CC}_{\mathrm{US}}} = \begin{cases} 0; \quad t=0 \\ \mathrm{q}_{t-1}^{\text{TOT, CC}_{\mathrm{US}}} + \mathrm{q}_t^{\text{CAP, CC}_{\mathrm{US}}}; \quad \forall t \neq 0 \end{cases} \tag{8}$$

$$0 \leq \mathrm{q}_t^{\text{TOT, CONV}_{\mathrm{US}}}; 0 \leq \mathrm{q}_t^{\text{TOT, CC}_{\mathrm{US}}} \tag{9}$$

$$0 \leq \mathrm{q}_t^{\mathrm{CONV_{US}}} \leq \mathrm{q}_t^{\text{TOT, CONV}_{\mathrm{US}}}; 0 \leq \mathrm{q}_t^{\mathrm{CC_{US}}} \leq \mathrm{q}_t^{\text{TOT, CC}_{\mathrm{US}}} \tag{10}$$

3.1.2 Downstream industry:

The downstream industry has the objective to maximise its discounted profits Π_t^{DS} for the entire optimisation period, expressed as the revenues $\mathcal{R}_t^{\mathrm{DS}}$ minus the incurred costs $\mathcal{C}_t^{\mathrm{DS}}$ in Eq. (11). As mentioned, the downstream industry can opt to produce traditionally without ($\mathrm{q}_t^{\mathrm{CONV_{DS}}}$) or with retrofitted carbon capture and storage ($\mathrm{q}_t^{\mathrm{CCS_{DS}}}$), and via the utilisation of carbon captured upstream ($\mathrm{q}_t^{\mathrm{CU_{DS}}}$). The downstream industry obtains revenues from selling the aggregated quantity of downstream product expressed by Eq. (12). The capital cost of Eq. (13) comprises the investment costs for a carbon utilisation installation, a conventional installation and retrofitted carbon capture, as expressed in Eq. (14). The operational cost of the downstream industry in (15) contain respectively: fuel costs for conventional production (also for the retrofitted carbon capture plant), variable costs related to CCS, variable costs related to CCU including transport, electricity and CO_2 feedstock costs and costs related to carbon pricing with ETS I and ETS II.

$$\max_{q_t^{\mathrm{DS}}} \sum_{t \in \Omega_{\mathrm{T^{OPT}}}} \Pi_t^{\mathrm{DS}} = \sum_{t \in \Omega_{\mathrm{T^{OPT}}}} \frac{1}{(1+\tau)^t} (\mathcal{R}_t^{\mathrm{DS}} - \mathcal{C}_t^{\mathrm{DS}}) \tag{11}$$

$$\mathcal{R}_t^{\mathrm{DS}} = \overbrace{\mathrm{p}^{\mathrm{DS}^*}(\mathrm{q}_t^{\mathrm{CONV_{DS}}} + \mathrm{q}_t^{\mathrm{CU_{DS}}} + \mathrm{q}_t^{\mathrm{CCS_{DS}}})}^{\text{Revenue from downstream product}} \tag{12}$$

$$\mathcal{C}_t^{\mathrm{DS}} = \mathrm{CAPEX}_t^{\mathrm{DS}} + \mathrm{OPEX}_t^{\mathrm{DS}} \tag{13}$$

$$\mathrm{CAPEX}_t^{\mathrm{DS}} = \overbrace{\frac{\mathrm{T^{OPT}} - t + 1}{\mathrm{T^{DS}}}}^{\text{Depreciation term}} \left(\overbrace{\mathrm{C}^{\mathrm{CAP,\ CU_{DS}}} \mathrm{q}_t^{\mathrm{CAP,\ CU_{DS}}} \Phi_t^{\mathrm{CU_{DS}}}}^{\text{CAPEX of RFNBO unit}} + \overbrace{\mathrm{C}^{\mathrm{CAP,\ CONV_{DS}}} \mathrm{q}_t^{\mathrm{CAP,\ CONV_{DS}}}}^{\text{CAPEX of conventional unit}} + \overbrace{\mathrm{C}^{\mathrm{CAP,\ CC_{DS}}} \mathrm{q}_t^{\mathrm{CAP,\ CC_{DS}}} (\chi^{\mathrm{CONV_{DS}}}(1 - \alpha^{\mathrm{CC_{DS}}}))}^{\text{CAPEX of retrofit carbon capture unit}} \right) \tag{14}$$

$$\begin{aligned}
\mathrm{OPEX}_t^{\mathrm{DS}} = & \overbrace{(\mathrm{q}_t^{\mathrm{CONV_{DS}}} + \mathrm{q}_t^{\mathrm{CCS_{DS}}}) \mathrm{E}^{\mathrm{CONV_{DS}}} \mathrm{C}_t^{\mathrm{fuel_{DS}}}}^{\text{Fuel costs for conventional product and product with capture}} + \overbrace{\mathrm{q}_t^{\mathrm{CCS_{DS}}} \chi^{\mathrm{CONV_{DS}}} (1 - \alpha^{\mathrm{CC_{DS}}})(\mathrm{C}_t^{\mathrm{E}} \mathrm{E}^{\mathrm{CC_{DS}}} + \mathrm{C^T} + \mathrm{C^S})}^{\text{Variable costs of product with capture and storage}} \\
& + \overbrace{\mathrm{q}_t^{\mathrm{CU_{DS}}} \Phi^{\mathrm{CU_{DS}}} (\mathrm{E}^{\mathrm{CU_{DS}}} \mathrm{C}_t^{\mathrm{E}} + \mathrm{C^T}/2)}^{\text{Transport and electricity costs of RFNBO product}} + \overbrace{\boldsymbol{\lambda}_{\mathbf{t}}^{\mathbf{CO_2}^*} \mathrm{q}_t^{\mathrm{CU_{DS}}} \Phi^{\mathrm{CU_{DS}}}}^{\text{Costs from } CO_2 \text{ commodity trading}} \\
& + \overbrace{\mathcal{Z}^{\mathrm{ETS}_{I,\mathrm{DS}}} (\mathrm{q}_t^{\mathrm{CCS_{DS}}} \alpha^{\mathrm{CC_{DS}}} \chi^{\mathrm{CONV_{DS}}} + \mathrm{q}_t^{\mathrm{CONV_{DS}}} \chi^{\mathrm{CONV_{DS}}}) \mathrm{C}_t^{\mathrm{ETS}_I}}^{\text{ETS I costs for (residual) emissions from conventional production and production with capture}} + \overbrace{\mathcal{Z}^{\mathrm{ETS}^*_{I,\mathrm{DS}}} \mathrm{q}_t^{\mathrm{CU_{DS}}} \chi^{\mathrm{CU_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_I}}^{\text{ETS I costs for residual emissions of RFNBO production}} \\
& + \overbrace{\mathcal{Z}^{\mathrm{ETS}_{II,\mathrm{DS}}} (\mathrm{q}_t^{\mathrm{CCS_{DS}}} + \mathrm{q}_t^{\mathrm{CONV_{DS}}}) \Phi^{\mathrm{USE_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_{II}}}^{\text{ETS II costs for fossil fuels}} + \overbrace{\mathcal{Z}^{\mathrm{ETS}^*_{II,\mathrm{DS}}} \mathrm{q}_t^{\mathrm{CU_{DS}}} \Phi^{\mathrm{USE_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_{II}}}^{\text{ETS II costs for RFNBO fuel}}
\end{aligned} \tag{15}$$

Again, production limits defined by the installed capacity are defined by Eq. (16)- (19):

$$\mathrm{q}_t^{\mathrm{TOT,\ CONV_{DS}}} = \begin{cases} \mathrm{Q}_{t=0}^{\mathrm{CONV_{DS}}}; & t = 0 \\ \mathrm{q}_{t-1}^{\mathrm{TOT,\ CONV_{DS}}} + \mathrm{q}_t^{\mathrm{CAP,\ CONV_{DS}}} - \mathrm{q}_t^{\mathrm{CAP,\ CC_{DS}}}; & \forall t \neq 0 \end{cases} \tag{16}$$

$$\mathrm{q}_t^{\mathrm{TOT,\ CC_{DS}}} = \begin{cases} 0; & t = 0 \\ \mathrm{q}_{t-1}^{\mathrm{TOT,\ CC_{DS}}} + \mathrm{q}_t^{\mathrm{CAP,\ CC_{DS}}}; & \forall t \neq 0 \end{cases} \tag{17}$$

$$q_t^{\text{TOT, CU}_{\text{DS}}} = \begin{cases} 0; & t = 0 \\ q_{t-1}^{\text{TOT, CU}_{\text{DS}}} + q_t^{\text{CAP, CU}_{\text{DS}}}; & \forall t \neq 0 \end{cases} \tag{18}$$

$$0 \leq q_t^{\text{CONV}_{\text{DS}}} \leq q_t^{\text{TOT, CONV}_{\text{DS}}}; 0 \leq q_t^{\text{CU}_{\text{DS}}} \leq q_t^{\text{TOT, CU}_{\text{DS}}}; 0 \leq q_t^{\text{CCS}_{\text{DS}}} \leq q_t^{\text{TOT, CC}_{\text{DS}}} \tag{19}$$

3.1.3 Consumers:

The consumers maximise their utility (U) by integrating their willingness to pay subtracted with the purchasing costs. This is expressed by Eq. (20) for the upstream product and Eq. (21) for the downstream product. In both cases, we assume a linear inverse demand curve to capture the implications of different ETS designs on changes in consumption. The slope and intercept (A and B) of this curve are independent of the time t.

$$\max_{q_t^{\text{US}}} \sum_{t \in \Omega_{\text{T}^{\text{OPT}}}} \text{U}^{\text{US}} = \sum_{t \in \Omega_{\text{T}^{\text{OPT}}}} \text{A}^{\text{US}} q_t^{\text{US}} - \text{B}^{\text{US}} {q_t^{\text{US}}}^2/2 - p_t^{\text{US}^*} q_t^{\text{US}} \tag{20}$$

$$\max_{q_t^{\text{DS}}} \sum_{t \in \Omega_{\text{T}^{\text{OPT}}}} \text{U}^{\text{DS}} = \sum_{t \in \Omega_{\text{T}^{\text{OPT}}}} \text{A}^{\text{DS}} q_t^{\text{DS}} - \text{B}^{\text{DS}} {q_t^{\text{DS}}}^2/2 - p_t^{\text{DS}^*} q_t^{\text{DS}} \tag{21}$$

3.1.4 Clearing constraints:

We impose market clearing conditions for the CO_2 commodity market in Eq. (22), the upstream product market in Eq. (23) and the downstream product market in Eq. (24). These determine the equilibrium prices to ensure a matching of demand and supply. In Eq. (22), the sold CO_2 quantities are related to the upstream pathway with CCU producing $q_t^{\text{CCU}_{\text{US}}}$ tonnes of product and $\chi^{\text{CONV}_{\text{US}}}(1 - \alpha^{\text{CC}_{\text{US}}})$ emissions per ton, and the downstream production pathway generating $q_t^{\text{CU}_{\text{DS}}}$ ton of RFNBO fuel and consuming $\Phi^{\text{CU}_{\text{DS}}}$ tonnes of CO_2 per ton of RFNBO product. For Eq. (23) the total demanded product (q_t^{US}) equals the products produced by the different production routes for each time step t. The same holds for the downstream product in Eq. (24).

$$q_t^{\text{CCU}_{\text{US}}} \chi^{\text{CONV}_{\text{US}}} (1 - \alpha^{\text{CC}_{\text{US}}}) = q_t^{\text{CU}_{\text{DS}}} \Phi^{\text{CU}_{\text{DS}}} \tag{22}$$

$$q_t^{\text{US}} = q_t^{\text{CONV}_{\text{US}}} + q_t^{\text{CCS}_{\text{US}}} + q_t^{\text{CCU}_{\text{US}}} \tag{23}$$

$$q_t^{\text{DS}} = q_t^{\text{CONV}_{\text{DS}}} + q_t^{\text{CU}_{\text{DS}}} + q_t^{\text{CCS}_{\text{DS}}} \tag{24}$$

3.2 Case study set-up

To investigate the extent to which the current EU ETS regulation economically disfavours the reuse of CO_2 under no or too low ETS II prices, we apply our modelling framework to a numerical case study using data of an upstream steel industry and a downstream refinery. The corresponding data can be found in Tab. III and IV of Appendix A, expressed in real terms to the base year, 2024. All other assumptions applied to this case study are listed as follows.

- Carbon capture is applied to the blast furnace in the blast furnace-basic oxygen furnace (BF-BOF) steel-making route. No electric arc furnace steelmaking is considered as the focus upstream is on capturing CO_2 in order to provide feedstock for e-fuel production downstream.
- The downstream industry covers the production of transportation fuels by conventional oil refinery processes, or switching to the production of RFNBO. In the latter case, they are 100% reliant on CO_2 from other industries (steel in this case). The e-fuel-producing technologies are assumed to be mature to deploy at large scales.
- Investments occur from 2025 onward, and take place till the year 2050. We assume that conventional legacy capacity is available. The year 2024, hence, functions as the base year resembling the existing conventional technology mix.
- The upstream industry is regarded to be twice the size of the downstream industry, i.e. the production (in tonnes of product per year) of the base year is twice as large upstream. This allows capturing CO_2 demand shortage downstream when product prices increase.
- Fossil CO_2 is considered for the production of RFNBO as such that ETS I allowances need to be surrendered on the traded CO_2 feedstock. Bio-based CO_2 or CO_2 that has been accounted for in an earlier stadium is not directly considered. Although this study only focuses on non-biogenic CO_2, some of the results can be extrapolated to biogenic CO_2 as well.
- The ETS I price is fixed (at 150 EUR/tCO_2) to compare the model outcomes with the Pareto-optimal production decisions. The EU ETS II price is expressed in the model as a fraction $\mathcal{F}_{\text{ETS II/I}}$ of the ETS I price.
- Electricity prices are assumed to be very low, equal to half of the TYNDP values [31]. This assumption has been made in order to capture the EU ETS effect on CCS and CCU production.
- All results are expressed in real terms. A real discount rate of 6% using 2024 as the base year is applied.

Two different ETS configurations, presented in Tab. I, are applied to the model and case study. They correspond to the previously mentioned 'Case 1: current projected regulation' and 'Case 2: proposed regulation', explained as well in Fig. 2. For both cases, ETS I allowances are paid on all emitted CO_2 upstream by default. Although the same holds for mineral oil refineries downstream, the RFNBO installation is not part of ETS I. Consequently, the existing ETS I regulation prescribes that captured carbon sent out of the upstream-covered ETS I installation should be backed by allowances by the upstream emitter. As a consequence, the RFNBO fuel is already been covered by ETS I, such that only conventional fuels are covered by ETS II allowances under the current regulation (Case 1) during their product-use phase. Alternatively, including the RFNBO installation in ETS I, would mean that no surrendering upstream is needed on the traded CO_2 feedstock. This is done in Case 2 as presented in Tab. I. To maintain the same emission coverage as in Case 1, ETS II is applied as well to RFNBOs produced with industrial-captured, non-biobased CO_2.

To be able to compare both cases in view of a socially optimal emission abatement strategy, a Pareto case is introduced as a reference. As shown by Tab. I, all emissions are covered by the same ETS I price at the point of emission. In fact, the Pareto case represents Case 2 where EU ETS I and II price levels are equalised.

TABLE I: Overview of ETS emission coverage for the two cases, as well as the Pareto Case.

Emission fractions		**Case 1**	**Case 2**	**Pareto case**
Upstream:	Non-captured exhaust emissions	ETS I	ETS I	ETS I
	Traded CO_2 commodity*	ETS I	-	-
	End-use emissions	-	-	-
Downstream:	Non-captured exhaust emissions	ETS I	ETS I	ETS I
	Exhaust emissions RFNBO production (if any)	-	ETS I	ETS I
	End-use emissions*	ETS II** *on* ***conventional*** *fuels*	ETS II** *on* ***all*** *fuels*	ETS I *on* ***all*** *fuels*

* These emission fractions cover in principle the same CO_2 molecules, such that double counting with carbon pricing is avoided in the case definition.
** $C^{ETS\ II} = \mathcal{F}_{ETS\ II/I} \cdot C^{ETS\ I}$, with $\mathcal{F}_{ETS\ II/I} \in [0,1.0]$

4. Results & Discussion

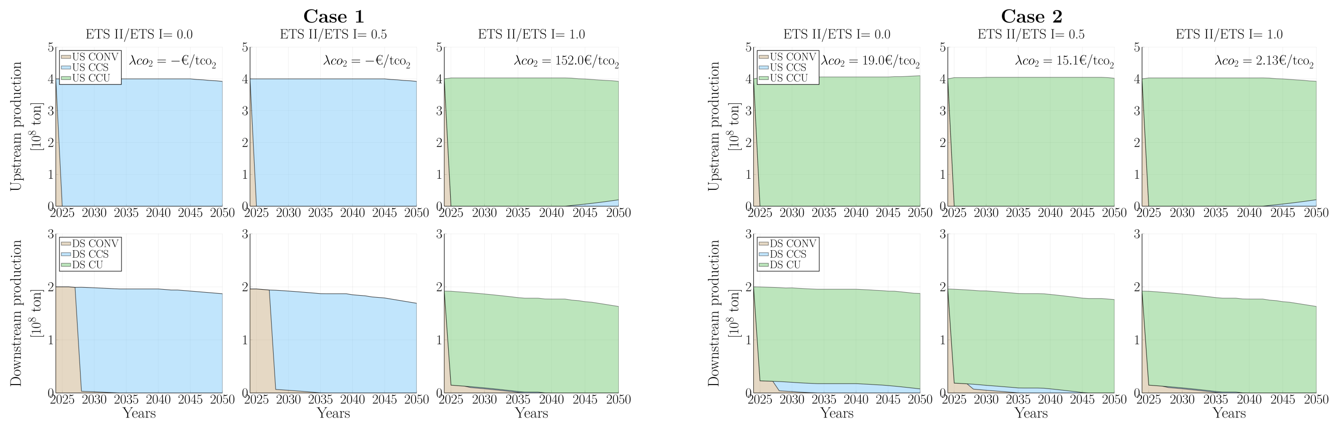
4.1 Numerical modelling results

Fig. 4 presents the numerical modelling outcomes expressing the yearly production quantities (2024-2050) for both Case 1 (4a) and Case 2 (4b), and for both the upstream (top rows) and downstream industry (bottom rows). The columns indicate the fraction between ETS II and ETS I prices ($\mathcal{F}_{ETS\ II/I}$) applied to each subplot. The yearly production quantities are expressed in tonnes of product. The total produced quantity can be derived from conventional (CONV), carbon capture with storage (CCS) and carbon (capture) utilisation (C(C)U) production routes. In case C(C)U takes place, an agreement on the CO_2 commodity trading price is established. The average price value is indicated with λ_{CO_2} on top of each ETS case in Fig. 4a and Fig. 4b.

Comparing both cases under equal ETS prices ($\mathcal{F}_{ETS\ II/I} = 1.0$) shows us that the same equilibrium solution is obtained regarding the technology decisions and related production quantities. The only difference is the CO_2 commodity trading price which increases by 150 euros per tonne of CO_2 in Case 1 relative to Case 2. This reflects the internalisation of the ETS I price in the CO_2 commodity price. Due to the harmonised EU ETS I & II prices, the downstream industry experiences the same carbon pricing burden on the CO_2 contained in fossil fuels (ETS II) as in RFNBOs (ETS I). The production route, here RFNBO production, that is least expensive also regarding other emissions during the production process, will be selected.

In Case 1, Fig. 4a, non-harmonised EU ETS prices clearly affect the investment and production outcomes. With EU ETS fractions of 0 and 0.5, fossil fuel production initially without and later with CCS, becomes more cost-attractive downstream than RFNBO production. The upstream industry follows by storing CO_2 instead of trading it. In fact, the ETS I price gets fully internalised again in the traded CO_2 price as contained in the RFNBO product, while ETS II prices applied to CO_2 of conventional fuels are now only a percentage of the EU ETS I, not providing enough stimulus for RFNBOs to be produced. Depending on the other cost parameters, for each year a threshold fraction $\overline{\mathcal{F}}_{ETS\ II/I}$ can be obtained at which the EU ETS II price is high enough to provide a sufficient economic incentive to produce RFNBOs. For this case study, $\overline{\mathcal{F}}_{ETS\ II/I}$ is 0.68 in 2050 and 0.87 in 2025, meaning that if the ETS II price is higher than 0.87 times the EU ETS I price, RFNBO production takes place from 2025 onward.

Case 2, in contrast, shows less dependence on ETS II. All subplots have C(C)U as the main production pathway in Fig. 4b. This is because all fuels in Case 2 are subject to ETS II pricing. Increasing the ETS II price will not alter the trade-offs between production decisions downstream or upstream and this case hence seems more robust against ETS price differentials. The carbon commodity trading price reduces from 19.2 EUR/tCO_2 to 2.1 EUR/tCO_2 on average when $\mathcal{F}_{\text{ETS II/I}}$ increases from 0 to 1.



(a) (b)

Fig. 4: Production quantities for the optimisation horizon (2025-2050) for (a) Case 1 (b) Case 2. The rows indicate the upstream or downstream production, the columns indicate an increase in the ETS II price going from 0 to 1.0 times the ETS I price level. CONV, CCS, C(C)U denote conventional, carbon capture with storage and carbon (capture with) utilisation respectively. US means upstream, DS means downstream.

4.2 Analytical result interpretation

Although the numerical case study confirms that a shift to CCS occurs under Case 1 with low ETS II prices, more generalisation and insights are needed to fully understand the ETS effect on CO_2 commodity trading. An analytical derivation allows us to generalise the modelling outcomes, enabling us to assess under which conditions CCU takes place. This derivation can be found in Appendix C where we derive trading bounds using the model formulation of Section 3. Those bounds allow us to find upper ($\overline{\lambda_t}^{CO_2}$) and lower limits ($\underline{\lambda_t}^{CO_2}$) on the carbon commodity trading price and the resulting trade of CO_2. The generated bounds can be interpreted as trade-offs made by producers between CO_2 trading and other production routes. The upper limit represents the maximum commodity price that the downstream firm is willing to pay such that they become indifferent between carbon utilisation or one of their other production routes. The lower limit likewise represents the minimum commodity price the upstream firm is willing to receive. The trade-off consists of OPEX and CAPEX parts, respectively indicating the difference in variable and fixed costs between two production routes[12]. Different trade-offs can be generated depending on the different production options available. Furthermore, as those bounds include ETS-related costs, it can help to better understand the relative effects of ETS I & II on the likeliness of RFNBO production.

[12]Note that a purely OPEX-driven bound can be found without solving the model. When a CAPEX term is included the bound can be derived from the modelling results after optimisation. This is further explained in Appendix C.

In this study, each industry, upstream and downstream, has three different production routes including one related to carbon utilisation, resulting in two trade-offs for each industry. There is the conventional production & utilisation trade-off (abbreviated as CONV-C(C)U) and the conventional production production with CCS & utilisation trade-off (abbreviated as CCS-C(C)U). This results in two upstream or lower bounds that express the minimum price on which the upstream industry decides to sell CO_2 feedstock, and two downstream or upper bounds expressing the maximum willingness to pay for CO_2 by the downstream industry. In Appendix C four equations, two upstream (Eq. (40),(41)) and two downstream (Eq. (40),(41)), associated with the CO_2 commodity trading bounds are established. Only one of the bounds at each industry sets the limits for CO_2 trading, that is the highest lower bound upstream and the lowest upper bound downstream. Those bounds are indicated as the 'active' bounds, as they represent the trade-off with the most competitive alternative. The remaining ones are the 'alternative' bounds.

Fig. 5 clarifies the trading bounds on CO_2 as applied to the numeric case study. It expresses both the active (solid lines) and alternative bounds (dashed lines) for CO_2 commodity trading under the three different values of $\mathcal{F}_{\text{ETS II/I}}$. The upstream bounds are indicated in a red colour, the downstream bounds are green. The horizontal axis expresses the evolution of those bounds through time. The vertical axis indicates the value of the bounds expressed in euros per tonne CO_2. From this figure, we can infer the conditions under which CO_2 commodity trading takes place together with the agreed price of the CO_2 commodity.

First, C(C)U production appearing in Fig. 4 can be explained by the relative bounds position in Fig. 5. In general, it holds that when the green solid upper bound downstream is higher than the red solid lower bound upstream, C(C)U takes place. That means that the willingness to pay for CO_2 by the downstream industry is higher than the minimum price the upstream industry wants to receive. Analytically this can be expressed by the threshold ETS fraction $\overline{\mathcal{F}}_{\text{ETS II/I}}$ obtained by Eq. (57) in Appendix C. For Case 1 and this case study, we can confirm that this occurs at the previously obtained fraction $\mathcal{F}_{\text{ETS II/I}}$ equal to 0.68 in 2050. For fractions equal to 0.0 and 0.5 the upper bound lies below the lower bound, making CO_2 trade and thus production with C(C)U infeasible. The optimisation script tells that in all ETS cases, the active (solid) upper bound belongs to the trade-off CU-CONV before 2033-2039, depending on the ETS case, and CU-CCS afterwards. Consequently, for too low $\mathcal{F}_{\text{ETS II/I}}$ or ETS II values, conventional production takes place first, followed by mainly CCS for the remaining years instead of RFNBO (CU) production. Phrased differently, when the upper bound falls below the lower bound, the best technology option is to first produce with the existing conventional refinery installation, later on followed by CCS when the ETS prices become too expensive. Fig. 4a confirms that finding.

For our proposed case, Case 2, the results are robust against ETS price differentials as the bounds do not change with changes in ETS II relative to ETS I. The technology trade-offs do not get affected as ETS II prices apply to all production routes. The upper bound is positioned higher than the lower bound so that RFNBO production will take place, confirmed by Fig. 4b. Note, that the lower bound upstream is negative in contrast to Case 1. As no ETS allowance surrendering applies to traded CO_2 feedstock, storage costs are higher than utilisation costs. Consequently, the upstream firm is willing to pay for CO_2.

Second, the eventual market price for CO_2 is indicated as well on Fig. 5 by the thin black line with green markers, again in relation to the ETS II price. This CO_2 trading price is obtained by extracting the dual of the market clearing constraint in Eq. (22) for each time step after solving the model. When CO_2 commodity trading takes place, a CO_2 price is generated that lies between the feasible range set by the lower and upper trading bounds.

By comparing both cases, one can tell that the CO_2 commodity has a higher price value in Case 1. The difference is 150 EUR/tCO_2 due to the internalisation of the ETS I price, confirmed earlier with Fig. 4. Likewise, we confirm that under harmonised ETS I and II prices ($\mathcal{F}_{\text{ETS II/I}} = 1$), Case 1 and Case 2 yield the same solution as the relative bound position, including the carbon commodity trading price, is the same.

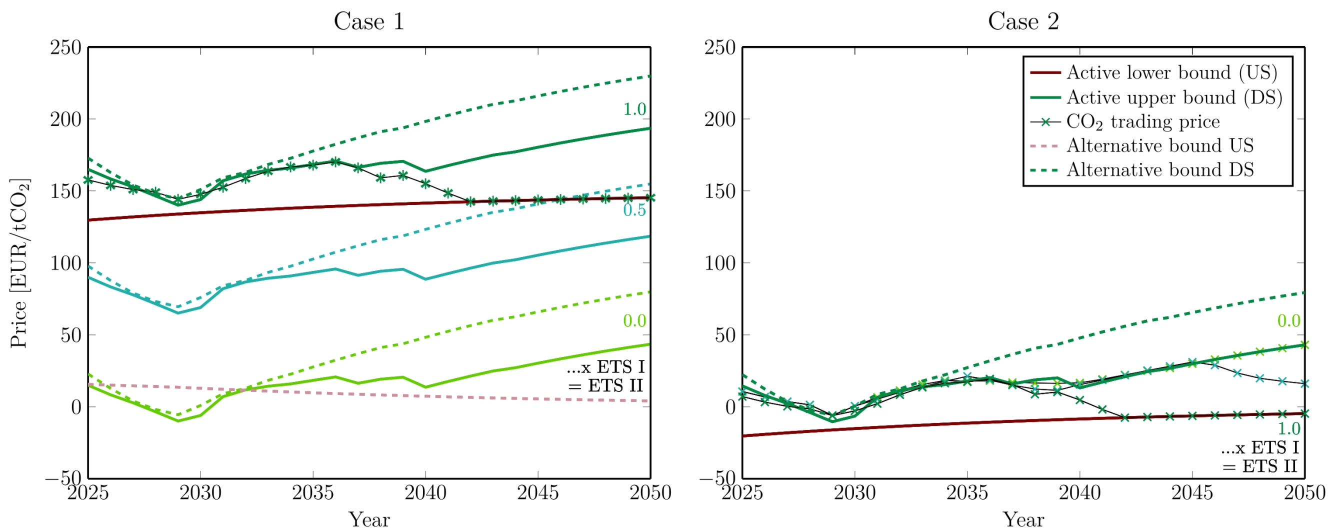


Fig. 5: Representation of the CO_2 commodity trading price (cross-marked line) including the upper and lower bounds (solid lines) and the alternative bounds (dashed lines) for each case. Different lines correspond to different ETS II price levels.

Lastly, we can analyse the ETS components of each bound. This provides more insight into how the ETS I & II influence the likeliness and dynamics of CO_2 commodity trading. The entire analysis can be found again under Appendix C (Fig. 7). We list the main findings as follows.

- In Case 2, a higher ETS I price **increases** the likelihood of CO_2 trading, due to an upward shift of the downstream bound as refinery processes (with or without CCS) are more emission-intensive and thus more affected by ETS I than RFNBO production. The upstream bound stays unaffected as CCS and CCU are both characterised by the same surrendering principles. Consequently, the EU ETS system stimulates the technology route with the lowest direct emissions.
- In Case 1, a higher ETS I price **decreases** the likelihood of CO_2 commodity trading as long as not all emissions downstream are properly covered by equally expensive ETS allowances. Put differently, as the CO_2 commodity trading price internalises the ETS I price, the willingness to pay downstream for CO_2 needs to scale proportionally with an increase of the ETS I price. That requires sufficient ETS II prices.
  - The absence of ETS II prices would mean that fewer CO_2 emissions are covered in the refinery case than in the RFNBO production case. The likelihood of RFNBO production decreases when the ETS I price increases.
  - In the presence of ETS II, the ETS II price level should be higher than the threshold $\overline{\mathcal{F}}_{\text{ETS II/I}}$. An increased ETS I price would require a lower price increase of ETS II, meaning that $\overline{\mathcal{F}}_{\text{ETS II/I}}$ declines (see Appendix C, Eq. (59)).

We mainly assessed the effect of the ETS II price relative to ETS I. However, it should be noted that other data inputs, e.g. a higher electricity price, could position the upper bound of Case 2 under the lower bound in Fig. 5. As such, CCS would dominate in Case 2. The same would hold in Case 1 unless the ETS II price becomes higher than ETS I. The interested reader finds the sensitivity analysis on other parameters in Appendix D.

We conclude this analytic section by stating that the bounds as expressed by the production trade-offs help to better interpret the impact of the ETS design on industrial decarbonisation outcomes. It could help policymakers to thoughtfully adjust the level of certain additional policy instruments, like tailored subsidies or taxes, to drive investment decisions in a certain direction.

4.3 Welfare implications

Finally, we would like to reflect on the relevance of our proposed regulatory case (Case 2) in terms of emission abatement and welfare compared to the current regulation (Case 1) and the Pareto-optimal abatement strategy. For that reason, Fig. 6 expresses the relative costs on the vertical axis in function of the abated emissions on the horizontal axis, both relative to a reference scenario with no carbon policies.

The economic loss on the y-axis is calculated by computing the total costs (CAPEX and OPEX) and by compensating for the changes in demand compared to the reference scenario. The horizontal axis represents the abated emissions that considers emissions from the upstream industry (electricity-related emissions, non-captured emissions) and downstream industry (electricity-related emissions, non-captured emissions, emissions due to fuel usage). Besides showing the results of both cases under varying ETS fractions $\mathcal{F}_{\text{ETS II/I}}$, a Pareto front has been created indicated by the dotted line. This Pareto front indicates the most cost-effective CO_2 reduction strategy for a certain level of abatement, such that no data points can be obtained under this line. It has been obtained by applying the same ETS price to all emission fractions (indicated in Tab. I) and by increasing the EU ETS price levels starting from 0 EUR/tCO_2. The higher this carbon allowance price, the more emissions are abated, and the higher the costs. For that reason, a parabolic curve is obtained. The 'black star'-marker indicates the Pareto situation with a uniform ETS price of 150 EUR/tCO_2 as applied to the ETS I parameter for all markers in Case 1 and 2.

We differentiate between two types of economic loss. These relate to (i) the consumption or production of sub-optimal levels of end-product and (ii) investments in sub-optimal production technologies.

The first economic loss factor occurs in both cases. Due to differences in ETS II and I prices the markers are located above the Pareto line. This effect is directly visible in Case 2. Lower incurred ETS costs lead to lower production upstream and higher production downstream than is socially optimal. A higher ETS fraction $\mathcal{F}_{\text{ETS II/I}}$ therefore leads to a smaller gap. An ETS fraction of 1 collides (in both cases) with the grey Pareto marker.

The second loss, related to sub-optimal technology decisions, is only visible in Case 1. For Case 1, the welfare gap is much higher than in Case 2. We can infer that this relates to a CCS lock-in effect downstream. As can be seen in Fig. 6 this CCS lock-in effect, or welfare gap, reduces after the identified fraction $\mathcal{F}_{\text{ETS II/I}}$ equal to 0.68. In fact, a transition phase from CCS to CCU occurs for fractions between 0.68 and 0.9, also reducing the amount of emissions. At a fraction close to 0.9, the threshold $\overline{\mathcal{F}}_{\text{ETS II/I}}$ is achieved for all the years between 2025-2050 in Case 1. Consequently, no CCS takes place and the small remaining optimality gap is now purely related to inefficient production and consumption levels.

In short, we state that Case 2 allows to obtain a closer to Pareto optimal outcome, irrespective of the ETS II levels. In contrast, Case 1 could yield a significant sub-optimal production scenario if no harmonisation of EU ETS prices takes place.

To highlight the inefficiency of the carbon pricing mechanism in Case 1, the solution of Case 2 with an ETS I price of 90 EUR/tCO_2 (grey markers) instead of 150 EUR/tCO_2 is plotted as well in Fig. 6. An ETS I price of 90 EUR/tCO_2 in Case 2 yields more or less the same level of abatement, but under lower relative costs as an ETS I allowance price of 150 EUR/tCO_2 in Case 1.

Appendix D contains more results related to the welfare distribution upstream and downstream. Besides, a reflection on the effect of the electricity carbon intensity levels in relation to RFNBO production is provided as well. It shows that under high carbon-intensive electricity generation, the CCS lock-in effect vanishes as CCS becomes less carbon-intensive in contrast to RFNBO production, the latter having a higher electricity demand.

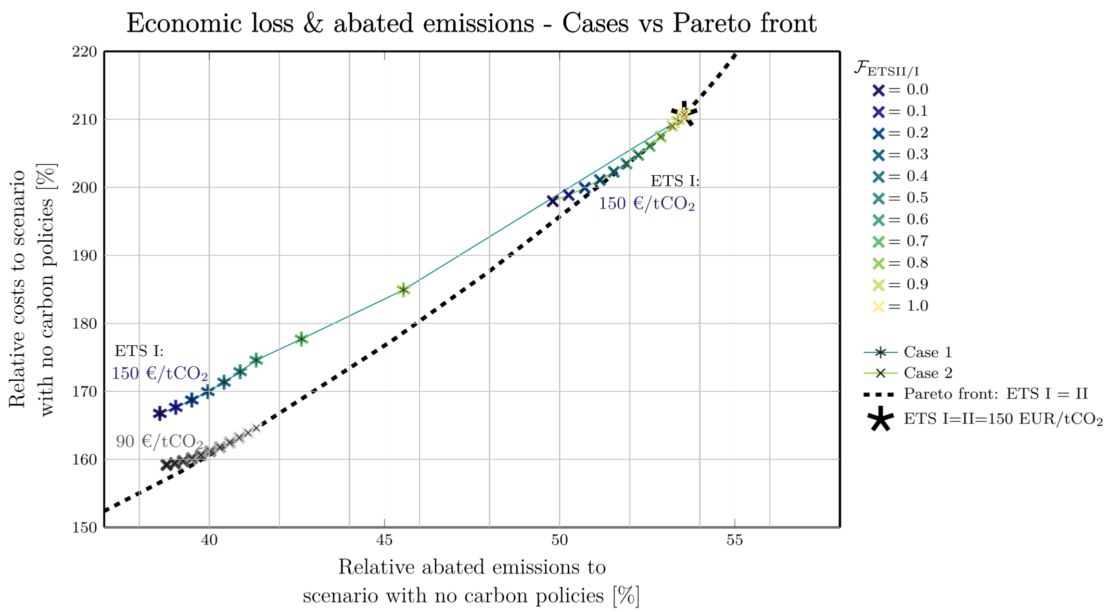


Fig. 6: Expressing the economic loss (incurred costs) and abated emissions in contrast to the Pareto optimal front. The closer to the front, the more optimal the results, here plotted for Case 1 and 2 under varying ETS II levels.

5. Conclusion

This paper unveils that the current EU ETS with non-harmonised ETS I & II prices distorts production and investment decisions in carbon capture storage (CCS) and utilisation (CCU), leading to inefficient emission abatement. We propose an alternative ETS I & II configuration that is more robust against those potential carbon pricing differentials. A stylised equilibrium framework developed in this study underpins the ETS distortion and has been applied in the context of the production of Renewable Fuels of Non-Biologic Origin (RFNBOs).

The current ETS regulation requires fossil CO_2 used in those e-fuels to be covered by ETS I allowances, while the CO_2 contained in conventional fuels will be subject from 2027 onward to ETS II prices. With no ETS II or ETS II prices lower than ETS I prices, the economic competitiveness of fossil fuels produced in refineries, hence, artificially increases compared to e-fuel production. The results of this study show that this could lock in too much CCS than what is socially optimal, possibly extending the operational time of high carbon-intensive refinery activities. The proposed ETS configuration is more consistent among fuel production processes by applying ETS II to all fossil fuels, including e-fuels or RFNBOs made from fossil-captured carbon. The ETS I surrendering mechanism on the traded CO_2 feedstock is hence disregarded. In contrast to the current ETS configuration, numeric results show that the level-playing field between CCS and CCU is restored in the proposed case, resulting in a more optimal solution in terms of welfare and emission abatement.

An analytical analysis applied to the modelling framework generalises the numerical results of this study, unravelling the ETS-related policy dynamics under each regulatory case. This analysis defines trading bounds, expressing the willingness to pay or sell CO_2 commodity with respect to the best alternative production route in relation to the ETS price dynamics. Besides, it unveils the carbon commodity trading price which internalises the ETS I price under the current regulation in contrast to the proposed regulation. Consequently, the current regulation does not provide a sufficient willingness to pay for the CO_2 commodity when ETS II prices are too low. Under constant ETS II prices, a higher ETS I price will thus decrease the likelihood of CO_2 commodity trading. Contrary, the proposed regulatory case is not influenced by ETS price differentials, nor by ETS II prices. Here, a higher ETS I price increases the likelihood of the process that emits the lowest amounts of CO_2. Under low-carbon intensive electricity production, this would be the RFNBO production route. Both regulatory cases yield the same production and investment outcome when ETS prices are harmonised. Only the carbon commodity trading price is different as it fully internalises the ETS I price under current regulation.

In short, we argue from a policy perspective that the proposed ETS configuration helps to create a better level-playing field between conventional production with or without carbon capture and storage, and, RFNBO production. A harmonisation of both ETSs is recommended when the current regulation is maintained. Furthermore, we support the use of a similar bounds analysis in stylised equilibrium modelling frameworks. It helps to get more insights from a regulatory point of view in understanding parameter interactions and regulatory pancaking. The analytic analysis could also help to better understand more detailed techno-economic modelling results.

We note that this paper just provides the introduction and initial exploration of a newly proposed ETS configuration. Our framework, however, is limited and more research is required to examine the detailed benefits and drawbacks of the proposal.

We acknowledge other shortcomings mainly related to the stylised nature of the modelling framework. Those involve rational agent behaviour and the purely deterministic foresight to make investment decisions. Furthermore, ETS prices are considered as given and hence do not capture feedback effects between sectors covered by ETS I or II. The framework could be extended emphasising different industry configurations, ETS configurations, support instruments (e.g. subsidies), and other technologies such as electricity or hydrogen-based production upstream. Considering the numerical case study, some of the applied parameters, like the low electricity prices, do not fully represent realistic parameter forecasts but are used to identify RFNBO production in order to unveil ETS dynamics. Higher electricity prices could make RFNBO production non-profitable in certain EU regions so that the ETS distortion fades under current regulations.

One main shortcoming of this study is that it primarily addresses CO_2 derived from industries that apply fossil energy sources. Nevertheless, including biogenic CO_2 could have a large influence on the investment results. Under the current regulation, biogenic CO_2 commodity could be cheaper as no ETS credits need to be surrendered in contrast to the CO_2 coming from a fossil-based industry as dealt with in this paper. The marginal carbon capture cost of the BECC plant would be reflected in this biogenic CO_2 feedstock price. A cheaper CO_2 commodity price would promote carbon utilisation downstream. To overcome this shortcoming, future research could focus more on bio-derived CO_2 for RFNBO production or the competition with biofuels and BECCS. Here, it becomes interesting to analyse how industries invest in carbon utilisation technologies in combination with the imposed EU quotas for RFNBOs and biofuels as well as negative emission pricing [7].

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Declaration of 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.

CRediT authorship contribution statement

Flore Verbist: Conceptualization; Methodology; Formal Analysis; Validation; Visualisation; Writing - original draft. **Jelle Meus:** Conceptualisation; Methodology; Writing - review & editing. **Jorge Andrés Moncada:** Conceptualisation; Writing - review & editing. **Erik Delarue:** Writing - review & editing. **Pieter Valkering:** Writing - review & editing

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Appendix A

Parameter values

TABLE II: Binary parameter values related to the ETS I & II for each case

	ETS I & II binary parameters					
Cases	$\mathcal{Z}^{\mathbf{ETS}_{I,\mathbf{US}}}$	$\mathcal{Z}^{\mathbf{ETS}_{I,\mathbf{DS}}}$	$\mathcal{Z}^{\mathbf{ETS}^*_{I,\mathbf{US}}}$	$\mathcal{Z}^{\mathbf{ETS}^*_{I,\mathbf{DS}}}$	$\mathcal{Z}^{\mathbf{ETS}_{II}}$	$\mathcal{Z}^{\mathrm{ETS}^*_{II}}$
No carbon policies	0	0	0	0	0	0
Pareto Case	1	1	0	1	1	1
Case 1	1	1	1	0	1	0
Case 2	1	1	0	1	1	1

TABLE III: Time independent parameter values used in the optimisation script, expressed in real (non-discounted) terms.

Symbol	**Value**	**Unit**	**Description**	**Source**
$\mathrm{T}^{\mathrm{OPT}}$	26	yrs	Investment period	
$\mathrm{Q}_{t=0}^{\mathrm{CONV_{US}}}$	400,000,000	tpa (ton produced per annum)	Initial installed conventional capacity of upstream industry	
$\mathrm{Q}_{t=0}^{\mathrm{CONV_{DS}}}$	200,000,000	tpa (ton produced per annum)	Initial installed conventional capacity of downstream industry	
T^{US}	30	yrs	Lifetime upstream production facility	
T^{US}	30	yrs	Lifetime downstream production facility	
A^{US}	5942.7	€/ton	Intercept of demand curve for upstream product	
B^{US}	$1.37e^{-5}$	€/ton^2	Slope of the demand curve for upstream industry	
A^{DS}	12733.5	€/ton	Intercept of demand curve for downstream product	
B^{DS}	$5.94e^{-5}$	€/ton^2	Slope of demand curve for downstream product	
τ	0.06	-	Real discount rate, with the discount factor: $\frac{1}{(1+\tau)^t}$	
$\mathrm{C}^{\mathrm{CAP,\ CC_{US}}}$	920	€/tCO_2 captured pa	CAPEX of carbon capture installation for upstream industry per ton CO_2 captured	[32]
$\mathrm{C}^{\mathrm{CAP,\ CC_{DS}}}$	1936.63	€/tCO_2 captured pa	CAPEX of carbon capture installation for downstream industry per ton CO_2 captured	[33]
$\mathrm{C}^{\mathrm{CAP,\ CU_{DS}}}$	399.50	€/tCO_2 used pa	CAPEX of carbon utilisation installation for downstream industry per ton CO_2 utilised	[34]
$\mathrm{C}^{\mathrm{CAP,\ CONV_{US}}}$	644	€/tpa	CAPEX of conventional installation for upstream industry per ton production	[35]
$\mathrm{C}^{\mathrm{CAP,\ CONV_{DS}}}$	790	€/tpa	CAPEX of conventional installation for downstream industry per ton production	[36]
C^{S}	11	€/tCO_2	Cost of CO_2 storage	[37]
C^{T}	21	€/tCO_2	Cost of CO_2 transport	[37]
$\mathrm{E}^{\mathrm{CONV_{US}}}$	3055	kWh/ton	Fossil fuel consumption to produce 1 ton of upstream product with conventional installation	[38]
$\mathrm{E}^{\mathrm{CC_{US}}}$	286	kWh/tCO_2	Electricity consumption to capture 1 ton of CO_2 by upstream industry	[32]
$\mathrm{E}^{\mathrm{CC_{DS}}}$	166	kWh/tCO_2	Electricity consumption to capture 1 ton of CO_2 by downstream industry	[34]
$\mathrm{E}^{\mathrm{CU_{DS}}}$	9829	kWh/tCO_2	Electricity consumption to purify and process 1 ton of CO_2 to convert it in downstream product (incl. electricity for hydrogen production)	[33]
$\mathrm{E}^{\mathrm{CONV_{DS}}}$	14290	kWh/ton	Fossil fuel consumption to produce 1 ton of downstream product with conventional installation	[39]
$\Phi^{\mathrm{CU_{DS}}}$	3.2	tCO_2/p.u.	Amount of tonnes CO_2 required to produce 1 ton of downstream product	[33]
$\Phi^{\mathrm{USE_{DS}}}$	3.2	tCO_2/ton	Amount of CO_2 emitted after combustion of jet fuel	[40]
$\alpha^{\mathrm{CC_{US}}}$	0.3	fraction	Upstream residual emission fraction after capture send to the atmosphere	[41]
$\alpha^{\mathrm{CC_{DS}}}$	0.67	fraction	Downstream residual emission fraction after capture send to the atmosphere	[34], [42]
$\chi^{\mathrm{CONV_{US}}}$	2.0	tCO_2/ton	CO_2 emitted by the conventional process to produce 1 ton of upstream product	[32]
$\chi^{\mathrm{CONV_{DS}}}$	2.5	tCO_2/ton	CO_2 emitted by the conventional process to produce 1 ton of downstream product	[34], [42]
$\chi^{\mathrm{CU_{DS}}}$	0.01	tCO_2/ton	CO_2 emitted with CO_2 utilisation process to produce 1 ton of downstream product	[33] [43]

TABLE IV: Time dependent parameter values used in the optimisation script, expressed in real (non-discounted) terms.

Year	**Electricity cost [€/kWh]**	**Carbon intensity electricity [kgCO_2e/kWh]**	**Kerosene [€/kWh]**	**Coal [€/kWh]**	**Crude oil [€/kWh]**	**Carbon credit price [€/tCO_2]**
Source(s)	[31, 44]	[45]	[46]	[46]	[46]	[47]
2024	0.0195	0.024	0.05198	0.02305	0.03132	150.00
2025	0.021	0.024	0.05198	0.02305	0.03132	159.00
2026	0.0225	0.024	0.05198	0.02305	0.03132	168.54
2027	0.024	0.024	0.05198	0.02305	0.03132	178.65
2028	0.0255	0.024	0.05198	0.02305	0.03132	189.37
2029	0.027	0.017	0.05256	0.0112	0.03132	200.73
2030	0.02715	0.017	0.05256	0.0112	0.03132	212.78
2031	0.0273	0.017	0.05256	0.0112	0.03132	225.54
2032	0.02745	0.017	0.05256	0.0112	0.03132	239.08
2033	0.0276	0.017	0.05256	0.0112	0.03132	253.42
2034	0.02775	0.013	0.05137	0.01111	0.03096	268.63
2035	0.0279	0.013	0.05137	0.01111	0.03096	284.74
2036	0.02805	0.013	0.05137	0.01111	0.03096	301.83
2037	0.0282	0.013	0.05137	0.01111	0.03096	319.94
2038	0.02835	0.013	0.05137	0.01111	0.03096	339.14
2039	0.0285	0.010	0.05018	0.0112	0.03024	359.48
2040	0.0285	0.010	0.05018	0.0112	0.03024	381.05
2041	0.0285	0.010	0.05018	0.0112	0.03024	403.92
2042	0.0285	0.010	0.05018	0.0112	0.03024	428.15
2043	0.0285	0.010	0.05018	0.0112	0.03024	453.84
2044	0.0285	0.0086	0.049	0.01147	0.02952	481.07
2045	0.0285	0.0086	0.049	0.01147	0.02952	509.93
2046	0.0285	0.0086	0.049	0.01147	0.02952	540.53
2047	0.0285	0.0086	0.049	0.01147	0.02952	572.96
2048	0.0285	0.0086	0.049	0.01147	0.02952	607.34
2049	0.0285	0.0086	0.049	0.01147	0.02952	643.78

Appendix B

Equivalent Optimisation Problem

$$
\begin{aligned}
\max_{q_t^{\mathrm{US}}, q_t^{\mathrm{DS}}} \sum_{t\in\Omega_{\mathrm{T^{OPT}}}} \Pi_t = & \sum_{t\in\Omega_{\mathrm{T^{OPT}}}} \frac{1}{(1+\tau)^t} \left(\mathrm{A^{US}} \mathrm{q}_t^{\mathrm{US}} - \mathrm{B^{US}} {\mathrm{q}_t^{\mathrm{US}}}^2/2 + \mathrm{A^{DS}} \mathrm{q}_t^{\mathrm{DS}} - \mathrm{B^{DS}} {\mathrm{q}_t^{\mathrm{DS}}}^2/2 \right) \\
& - \sum_{t\in\Omega_{\mathrm{T^{OPT}}}} \frac{1}{(1+\tau)^t} \left(\overbrace{\frac{\mathrm{T^{OPT}} - t + 1}{\mathrm{T^{US}}}}^{\text{Depreciation term}} \left(\overbrace{\mathrm{C}^{\mathrm{CAP,\,CC_{US}}} \mathrm{q}_t^{\mathrm{CAP,CC_{US}}} \chi^{\mathrm{CONV_{US}}} (1-\alpha^{\mathrm{CC_{US}}})}^{\text{CAPEX or retrofit carbon capture unit}} + \overbrace{\mathrm{C}^{\mathrm{CAP,\,CONV_{US}}} \mathrm{q}_t^{\mathrm{CAP,\,CONV_{US}}}}^{\text{CAPEX conventional unit}} \right) \right. \\
& + \overbrace{\frac{\mathrm{T^{OPT}} - t + 1}{\mathrm{T^{DS}}}}^{\text{Depreciation term}} \left(\overbrace{\mathrm{C}^{\mathrm{CAP,\,CU_{DS}}} \mathrm{q}_t^{\mathrm{CAP,\,CU_{DS}}} \Phi_t^{\mathrm{CU_{DS}}}}^{\text{CAPEX of RFNBO unit}} + \overbrace{\mathrm{C}^{\mathrm{CAP,\,CONV_{DS}}} \mathrm{q}_t^{\mathrm{CAP,\,CONV_{DS}}}}^{\text{CAPEX of conventional unit}} + \right. \\
& \left. + \overbrace{\mathrm{C}^{\mathrm{CAP,\,CC_{DS}}} \mathrm{q}_t^{\mathrm{CAP,\,CC_{DS}}} (\chi^{\mathrm{CONV_{DS}}} (1-\alpha^{\mathrm{CC_{DS}}}))}^{\text{CAPEX of retrofit carbon capture unit}} \right) \\
& + \overbrace{(\mathrm{q}_t^{\mathrm{CONV_{US}}} + \mathrm{q}_t^{\mathrm{CC_{US}}}) \mathrm{E}^{\mathrm{CONV_{US}}} \mathrm{C}_t^{\mathrm{fuel_{US}}}}^{\text{Fuel costs for conventional product and product with capture}} + \overbrace{\mathrm{q}_t^{\mathrm{CC_{US}}} \mathrm{E}^{\mathrm{CC_{US}}} \chi^{\mathrm{CONV_{US}}} (1-\alpha^{\mathrm{CC_{US}}}) \mathrm{C}_t^{\mathrm{E}}}^{\text{Electricity cost for product with capture}} \\
& + \overbrace{\mathrm{q}_t^{\mathrm{CCS_{US}}} \chi^{\mathrm{CONV_{US}}} (1-\alpha^{\mathrm{CC_{US}}}) (\mathrm{C^T} + \mathrm{C^S})}^{\text{Transport \& storage costs for product with capture to storage}} + \overbrace{\mathrm{q}_t^{\mathrm{CCU_{US}}} \chi^{\mathrm{CONV_{US}}} (1-\alpha^{\mathrm{CC_{US}}}) (\mathrm{C^T}/2)}^{\text{Transport costs for product with capture to RFNBO}} \\
& + \overbrace{\mathcal{Z}^{\mathrm{ETS}_{I,\mathrm{US}}} (\mathrm{q}_t^{\mathrm{CC_{US}}} \alpha^{\mathrm{CC_{US}}} \chi^{\mathrm{CONV_{US}}} + \mathrm{q}_t^{\mathrm{CONV_{US}}} \chi^{\mathrm{CONV_{US}}}) \mathrm{C}_t^{\mathrm{ETS}_I}}^{\text{ETS I costs for (residual) emissions from conventional product and product with capture}} + \overbrace{\mathcal{Z}^{\mathrm{ETS}^*_{I,\mathrm{US}}} \mathrm{q}_t^{\mathrm{CCU_{US}}} \chi^{\mathrm{CONV_{US}}} (1-\alpha^{\mathrm{CC_{US}}}) \mathrm{C}_t^{\mathrm{ETS}_I}}^{\text{ETS I costs for transferred } \mathrm{CO_2} \text{ emissions}} \\
& + \overbrace{(\mathrm{q}_t^{\mathrm{CONV_{DS}}} + \mathrm{q}_t^{\mathrm{CCS_{DS}}}) \mathrm{E}^{\mathrm{CONV_{DS}}} \mathrm{C}_t^{\mathrm{fuel_{DS}}}}^{\text{Fuel costs for conventional product and product with capture}} + \overbrace{\mathrm{q}_t^{\mathrm{CCS_{DS}}} \chi^{\mathrm{CONV_{DS}}} (1-\alpha^{\mathrm{CC_{DS}}}) (\mathrm{C}_t^{\mathrm{E}} \mathrm{E}^{\mathrm{CC_{DS}}} + \mathrm{C^T} + \mathrm{C^S})}^{\text{Variable costs of product with capture and storage}} \\
& + \overbrace{\mathrm{q}_t^{\mathrm{CU_{DS}}} \Phi^{\mathrm{CU_{DS}}} (\mathrm{E}^{\mathrm{CU_{DS}}} \mathrm{C}_t^{\mathrm{E}} + \mathrm{C^T}/2)}^{\text{Transport and electricity costs of RFNBO product}} \\
& + \overbrace{\mathcal{Z}^{\mathrm{ETS}_{I,\mathrm{DS}}} (\mathrm{q}_t^{\mathrm{CCS_{DS}}} \alpha^{\mathrm{CC_{DS}}} \chi^{\mathrm{CONV_{DS}}} + \mathrm{q}_t^{\mathrm{CONV_{DS}}} \chi^{\mathrm{CONV_{DS}}}) \mathrm{C}_t^{\mathrm{ETS}_I}}^{\text{ETS I costs for (residual) emissions from conventional production and production with capture}} + \overbrace{\mathcal{Z}^{\mathrm{ETS}^*_{I,\mathrm{DS}}} \mathrm{q}_t^{\mathrm{CU_{DS}}} \chi^{\mathrm{CU_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_I}}^{\text{ETS I costs for residual emissions of RFNBO production}} \\
& \left. + \overbrace{\mathcal{Z}^{\mathrm{ETS}_{II,\mathrm{DS}}} (\mathrm{q}_t^{\mathrm{CCS_{DS}}} + \mathrm{q}_t^{\mathrm{CONV_{DS}}}) \Phi^{\mathrm{USE_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_{II}}}^{\text{ETS II costs for fossil fuels}} + \overbrace{\mathcal{Z}^{\mathrm{ETS}^*_{II,\mathrm{DS}}} \mathrm{q}_t^{\mathrm{CU_{DS}}} \Phi^{\mathrm{USE_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_{II}}}^{\text{ETS II costs for RFNBO fuel}} \right)
\end{aligned}
\tag{25}
$$

Appendix C

Bounds on CO_2 commodity Trading Price

C.1 Upper bound by downstream industry

To derive the upper bound of the price on CO_2, the Lagrangian can be used as expressed by (26). It corresponds to the objective ($\mathrm{OBJ^{DS}}$) defined in (11) (further specified by the expressions in (12)- (15)) with the addition of the constraints and expressions of Eq. (16) -(19) and (24) multiplied by their Lagrangian multipliers ($\gamma_t, \beta_t, \delta_t, \epsilon_t$). A recursive formulation appears due to the integration of Eq. (16) - (18).

$$\mathcal{L}_t^{\text{DS}}[q_t^{\text{DS}}, q_t^{\text{CONV}_{\text{DS}}}, q_t^{\text{CU}_{\text{DS}}}, q_t^{\text{CCS}_{\text{DS}}}, q_t^{\text{CAP, CU}_{\text{DS}}}, q_t^{\text{CAP, CC}_{\text{DS}}}, q_t^{\text{CAP, CONV}_{\text{DS}}}, \gamma_t, \beta_t, \delta_t, \epsilon_t] = -\text{OBJ}^{\text{DS}} + \sum_1^t \tag{26}$$

$$\Big(\gamma_t(q_t^{\text{DS}} - q_t^{\text{CU}_{\text{DS}}} - q_t^{\text{CONV}_{\text{DS}}} - q_t^{\text{CCS}_{\text{DS}}}) + \beta_t(q_t^{\text{CU}_{\text{DS}}} - q_t^{\text{CAP, CU}_{\text{DS}}} - q_{t-1}^{\text{CAP, CU}_{\text{DS}}} - ... - q_1^{\text{CAP, CU}_{\text{DS}}}) +$$

$$\delta_t(q_t^{\text{CONV}_{\text{DS}}} - (q_t^{\text{CAP, CONV}_{\text{DS}}} - q_t^{\text{CAP, CC}_{\text{DS}}}) - (q_{t-1}^{\text{CAP, CONV}_{\text{DS}}} - q_{t-1}^{\text{CAP, CC}_{\text{DS}}}) - ... - (q_1^{\text{CAP, CU}_{\text{DS}}} - q_1^{\text{CAP, CC}_{\text{DS}}})) - Q_{t=0}^{\text{CONV}_{\text{DS}}}) +$$

$$\epsilon_t(q_t^{\text{CCS}_{\text{DS}}} - q_t^{\text{CAP, CC}_{\text{DS}}} - q_{t-1}^{\text{CAP, CC}_{\text{DS}}} - ... - q_1^{\text{CAP, CC}_{\text{DS}}})\Big)$$

The derivative of the Lagrangian can be derived for each of the primal and dual variables, such that four dual stationarity conditions appear in Eq. (27)-(30) and seven primal stationarity conditions in Eq. (31)-(37), each with the orthogonal relationship ($\perp$).

$$\forall t : \gamma_t = \text{free} \quad \perp \quad \frac{\partial \mathcal{L}}{\partial \gamma_t} = \text{q}_t^{\text{DS}} = \text{q}_t^{\text{CU}_{\text{DS}}} + \text{q}_t^{\text{CCS}_{\text{DS}}} + \text{q}_t^{\text{CONV}_{\text{DS}}} \tag{27}$$

$$\forall t : 0 \leq \beta_t \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial \beta_t} = \text{q}_t^{\text{TOT, CU}_{\text{DS}}} - \text{q}_t^{\text{CU}_{\text{DS}}} \tag{28}$$

$$\forall t : 0 \leq \delta_t \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial \delta_t} = \text{q}_t^{\text{TOT, CONV}_{\text{DS}}} - \text{q}_t^{\text{CONV}_{\text{DS}}} \tag{29}$$

$$\forall t : 0 \leq \epsilon_t \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial \epsilon_t} = \text{q}_t^{\text{TOT, CC}_{\text{DS}}} - \text{q}_t^{\text{CC}_{\text{DS}}} \tag{30}$$

From equation (31) one can derive that $\gamma_t = \text{p}_t^{\text{DS}^*}$ when downstream production takes place ($0 < q_t^{\text{DS}}$). As such γ_t is already replaced in equations (32), (34) and (33) below.

$$\forall t : 0 \leq q_t^{\text{DS}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\text{DS}}} = \gamma_t - \text{p}_t^{\text{DS}^*} \tag{31}$$

The orthogonal relationships in (32), (34) and (33) signify that no production would occur ($q_t^{\cdot\cdot\text{DS}} = 0$) when the costs are higher than the income from selling a unit of product produced with a certain production route.

$$\forall t : 0 \leq q_t^{\text{CU}_{\text{DS}}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\text{CU}_{\text{DS}}}} = (\frac{\text{C}^{\text{T}}}{2} + \text{C}_t^{\text{E}}\text{E}^{\text{CU}_{\text{DS}}})\Phi^{\text{CU}_{\text{DS}}} + \mathcal{Z}^{\text{ETS}^*_{II,\text{DS}}}\Phi^{\text{USE}_{\text{DS}}}\text{C}_t^{\text{ETS}_{II}} + \tag{32}$$

$$\mathcal{Z}^{\text{ETS}^*_{I,\text{DS}}}\text{q}_t^{\text{CU}_{\text{DS}}}\chi^{\text{CU}_{\text{DS}}}\text{C}_t^{\text{ETS}_I} + \lambda^{\text{CO}_2}\Phi^{\text{CU}_{\text{DS}}} - \text{p}_t^{\text{DS}^*} + \beta_t$$

$$\forall t : 0 \leq q_t^{\text{CONV}_{\text{DS}}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\text{CONV}_{\text{DS}}}} = \text{E}^{\text{CONV}_{\text{DS}}}\text{C}_t^{\text{fuel}_{\text{DS}}} + \mathcal{Z}^{\text{ETS}_{I,\text{DS}}}\text{q}_t^{\text{CONV}_{\text{DS}}}\chi^{\text{CONV}_{\text{DS}}}\text{C}_t^{\text{ETS}_I} + \mathcal{Z}^{\text{ETS}_{II,\text{DS}}}\text{q}_t^{\text{CONV}_{\text{DS}}}\Phi^{\text{USE}_{\text{DS}}}\text{C}_t^{\text{ETS}_{II}} - \text{p}_t^{\text{DS}^*} + \delta_t \tag{33}$$

$$\forall t : 0 \leq q_t^{\text{CCS}_{\text{DS}}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\text{CCS}_{\text{DS}}}} = \text{E}^{\text{CONV}_{\text{DS}}}\text{C}_t^{\text{fuel}_{\text{DS}}} + \text{E}^{\text{CC}_{\text{DS}}}\chi^{\text{CONV}_{\text{DS}}}(1-\alpha^{\text{CC}_{\text{DS}}})(\text{C}_t^{\text{E}} + \text{C}^{\text{S}} + \text{C}^{\text{T}}) + \mathcal{Z}^{\text{ETS}_{I,\text{DS}}}\text{q}_t^{\text{CONV}_{\text{DS}}}\chi^{\text{CONV}_{\text{DS}}}(1-\alpha^{\text{CC}_{\text{DS}}})\text{C}_t^{\text{ETS}_I} + \mathcal{Z}^{\text{ETS}_{II,\text{DS}}}\text{q}_t^{\text{CCS}_{\text{DS}}}\Phi^{\text{USE}_{\text{DS}}}\text{C}_t^{\text{ETS}_{II}} - \text{p}_t^{\text{DS}^*} + \epsilon_t \tag{34}$$

The stationary constraints related to the investment (CAP) variables are expressed in Eq. (35)-(37). For one particular point in time t, the investment decisions depend on the Lagrangian multipliers of the future time steps due to the recurrent formulation. The sum of those multipliers should be equal to the capital expenditures at time t when investment takes place. This allows to recover the investment costs.

$$\forall t : 0 \leq q_t^{\text{CAP,CU}_{\text{DS}}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\text{CAP, CU}_{\text{DS}}}} = \frac{\text{T}^{\text{OPT}} - t + 1}{\text{T}^{\text{DS}}}\text{C}^{\text{CAP, CU}_{\text{DS}}}\Phi_t^{\text{CU}_{\text{DS}}} - \beta_t - \beta_{t+1} - ... - \beta_{T^{\text{OPT}}} \tag{35}$$

$$\forall t : 0 \leq q_t^{\text{CAP,CC}_{\text{DS}}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\text{CAP,CC}_{\text{DS}}}} = \frac{\text{T}^{\text{OPT}} - t + 1}{\text{T}^{\text{DS}}}\text{C}^{\text{CAP, CC}_{\text{DS}}}\chi^{\text{CONV}_{\text{DS}}}(1-\alpha^{\text{CC}_{\text{DS}}}) - \epsilon_t - \epsilon_{t+1} - ... - \epsilon_{T^{\text{OPT}}} + (\delta_t + \delta_{t+1} + ... + \delta_{T^{\text{OPT}}}) \tag{36}$$

$$\forall t : 0 \leq q_t^{\text{CAP,CONV}_{\text{DS}}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\text{CAP,CONV}_{\text{DS}}}} = \frac{\text{T}^{\text{OPT}} - t + 1}{\text{T}^{\text{DS}}}\text{C}^{\text{CAP, CONV}_{\text{DS}}} - \delta_t - \delta_{t+1} - ... - \delta_{T^{\text{OPT}}} \tag{37}$$

If we assume that at time t: $q_t^{\text{CAP,CU}_{\text{DS}}} > 0$, meaning that investment and production in carbon utilisation installations could take place, it will result in $\beta_t + \beta_{t+1} + ... + \beta_{T^{\text{OPT}}} = \frac{\text{T}^{\text{OPT}}-t+1}{\text{T}^{\text{DS}}}\Phi^{\text{CU}_{\text{DS}}}\text{C}^{\text{CAP, CU}_{\text{DS}}}$ (capital expenditures of period t). As we want to get an expression for β_t only to derive the upper bound in Eq. (32), an expression for the other β's should be found first.

This can be obtained by first deriving an expression for $\beta_{T^{\text{OPT}}}$ when $t = \text{T}^{\text{OPT}}$. Here we know from (35) that $\beta_{T^{\text{OPT}}}$ should be smaller or equal to the capital cost of the last period T^{OPT}, which is: $\frac{\text{T}^{\text{OPT}}-\text{T}+1}{\text{T}^{\text{DS}}}\Phi^{\text{CU}_{\text{DS}}}\text{C}^{\text{CAP, CU}_{\text{DS}}}$. Consequently, Eq. (32) says that for $q_{t=T^{\text{OPT}}}^{\text{CU}_{\text{DS}}} > 0$ the equilibrium price of the downstream product, equalises the operational expenditures including some marginal rent which is smaller than or equal to the capital expenditures of period T^{OPT}. $\beta_{T^{\text{OPT}}}$ is zero when RFNBO production does not occur at full capacity during that time step, which is when the lagrangian in Eq. (28) is larger than zero. Due to the uncertainty about parameter $\beta_{T^{\text{OPT}}}$, the other β_t's are also not known before solving the model. We do know that each of those β_t's obtain a value that lies between zero and $\frac{\text{T}^{\text{OPT}}-\text{t}+1}{\text{T}^{\text{DS}}}\Phi^{\text{CU}_{\text{DS}}}\text{C}^{\text{CAP, CU}_{\text{DS}}}$. We also know that when at time t investment in CU occurs, the sum of all β_t's that follow, including β_t, should equal the capital expenditures per unit of product of time t. For that reason we express β_t with Eq. (38):

$$\beta_t = x_t \overbrace{\frac{\mathrm{T}^{\mathrm{OPT}} - t + 1}{\mathrm{T}^{\mathrm{DS}}}}^{x_t^{\mathrm{CU}}} \Phi^{\mathrm{CU_{DS}}} \mathrm{C}^{\mathrm{CAP,\ CU_{DS}}} = x_t^{\mathrm{CU}} \Phi^{\mathrm{CU_{DS}}} \mathrm{C}^{\mathrm{CAP,\ CU_{DS}}}; \quad x_t \in [0,1] \tag{38}$$

This allows us to express the upper bound of λ^{CO_2} in Eq. (56) as:

$$\lambda_t^{\mathrm{CO_2}} \leq \left(\mathrm{p}^{\mathrm{DS}^*} - x_t^{\mathrm{CU}} \Phi^{\mathrm{CU_{DS}}} \mathrm{C}^{\mathrm{CAP,\ CU_{DS}}} - \left(\left(\frac{\mathrm{C}^{\mathrm{T}}}{2} + \mathrm{C}_t^{\mathrm{E}} \mathrm{E}^{\mathrm{CU_{DS}}} \right) \Phi^{\mathrm{CU_{DS}}} \right) - \left(\mathcal{Z}^{\mathrm{ETS}^*_{I,\mathrm{DS}}} \mathrm{q}_t^{\mathrm{CU_{DS}}} \chi^{\mathrm{CU_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_I} + \mathcal{Z}^{\mathrm{ETS}^*_{II,\mathrm{DS}}} \Phi^{\mathrm{USE_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_{II}} \right) \right) \frac{1}{\Phi^{\mathrm{CU_{DS}}}} \tag{39}$$

Eq. (39) still contains the equilibrium price of the downstream product, which is unknown at first sight. However, this can be interpreted as the marginal cost of the best production alternative besides carbon utilisation, so conventional production as derived from Eq. (33), (37) or carbon capture & storage with Eq. (34), (36). The value for $\mathrm{p}^{\mathrm{DS}^*}$ is obtained by first finding an expression for δ_t and ϵ_t in a similar way as done for β_t. This leads to the following to trade-offs:

- In case the best production alternative would be conventional production, this would result in (40):

$$\overline{\lambda_{\mathrm{t}}}^{\mathrm{CO_2}} = \overbrace{\frac{1}{\Phi^{\mathrm{CU_{DS}}}}}^{\substack{\text{Normalised per tCO2} \\ \text{used per ton product}}} \left(\overbrace{\left(x_t^{\mathrm{CONV}} \mathrm{C}^{\mathrm{CAP,\ CONV_{DS}}} - x_t^{\mathrm{CU}} \mathrm{C}^{\mathrm{CAP,\ CU_{DS}}} \Phi_t^{\mathrm{CU_{DS}}} \right)}^{\text{Difference CAPEX of conventional unit and carbon utilisation unit}} + \overbrace{\left(\mathrm{E}^{\mathrm{CONV_{DS}}} \mathrm{C}_t^{\mathrm{fuel_{DS}}} - \left(\frac{\mathrm{C}^{\mathrm{T}}}{2} + \mathrm{C}_t^{\mathrm{E}} \mathrm{E}^{\mathrm{CU_{DS}}} \right) \Phi^{\mathrm{CU_{DS}}} \right)}^{\substack{\text{Difference OPEX of conventional production} \\ \text{and carbon utilisation excluding carbon pricing}}} + \overbrace{\left(\left(\mathcal{Z}^{\mathrm{ETS}_{I,\mathrm{DS}}} \chi^{\mathrm{CONV_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_I} + \mathcal{Z}^{\mathrm{ETS}_{II,\mathrm{DS}}} \Phi^{\mathrm{USE_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_{II}} \right) - \left(\mathcal{Z}^{\mathrm{ETS}^*_{I,\mathrm{DS}}} \chi^{\mathrm{CU_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_I} + \mathcal{Z}^{\mathrm{ETS}^*_{II,\mathrm{DS}}} \Phi^{\mathrm{USE_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_{II}} \right) \right)}^{\text{Difference carbon pricing of conventional production and carbon utilisation}} \right) \tag{40}$$

  This expression signifies the difference between the fixed and variable costs of conventional production and carbon utilisation. Note that in our case due to the presence of conventional assets at time $t = 0$, the capital expenditures of the conventional refineries are removed from Eq. (40). This lowers the upper bound on the CO_2 commodity price.

- In case the best production alternative would be carbon capture & storage production, this would result in (41):

$$\overline{\lambda_{\mathrm{t}}}^{\mathrm{CO_2}} = \overbrace{\frac{1}{\Phi^{\mathrm{CU_{DS}}}}}^{\substack{\text{Normalised per tCO2} \\ \text{used per ton product}}} \left(\overbrace{\left(x_t^{\mathrm{CC}} \left(\mathrm{C}^{\mathrm{CAP,\ CC_{DS}}} \chi^{\mathrm{CONV_{DS}}} (1 - \alpha^{\mathrm{CC_{DS}}}) + \mathrm{C}^{\mathrm{CAP,\ CONV_{DS}}} \right) - x_t^{\mathrm{CU}} \mathrm{C}^{\mathrm{CAP,\ CU_{DS}}} \Phi_t^{\mathrm{CU_{DS}}} \right)}^{\text{CAPEX of carbon capture unit}} + \overbrace{\left(\left(\mathrm{E}^{\mathrm{CONV_{DS}}} \mathrm{C}_t^{\mathrm{fuel_{DS}}} + \chi^{\mathrm{CONV_{DS}}} (1 - \alpha^{\mathrm{CC_{DS}}}) (\mathrm{C}_t^{\mathrm{E}} \mathrm{E}^{\mathrm{CC_{DS}}} + \mathrm{C}^{\mathrm{S}} + \mathrm{C}^{\mathrm{T}}) \right) - \left(\frac{\mathrm{C}^{\mathrm{T}}}{2} + \mathrm{C}_t^{\mathrm{E}} \mathrm{E}^{\mathrm{CU_{DS}}} \right) \Phi^{\mathrm{CU_{DS}}} \right)}^{\text{Difference OPEX of CCS and carbon utilisation}} + \overbrace{\left(\left(\mathcal{Z}^{\mathrm{ETS}_{I,\mathrm{DS}}} \chi^{\mathrm{CONV_{DS}}} \alpha^{\mathrm{CC_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_I} + \mathcal{Z}^{\mathrm{ETS}_{II,\mathrm{DS}}} \Phi^{\mathrm{USE_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_{II}} \right) - \left(\mathcal{Z}^{\mathrm{ETS}^*_{I,\mathrm{DS}}} \chi^{\mathrm{CU_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_I} + \mathcal{Z}^{\mathrm{ETS}^*_{II,\mathrm{DS}}} \Phi^{\mathrm{USE_{DS}}} \mathrm{C}_t^{\mathrm{ETS}_{II}} \right) \right)}^{\text{Difference carbon pricing of CCS and carbon utilisation}} \right) \tag{41}$$

This expression signifies the difference between the fixed and variable costs of CCS production and carbon utilisation. The capex of conventional installations could be removed when existing assets are present at time $t = 0$.

Note that we ignored the discount rate τ in the bounds-derivation. Opex-related terms are multiplied with the discount factor $\frac{1}{(1+\tau)^t}$, while for capex-related terms this depends on the β_t's that take a value other than zero. For that reason, x_t could slightly deviate from the interval [0,1].

C.2 Lower bound by upstream industry

In a similar way as the upper bound, the lower bound on CO_2 determined by the upstream industry can be derived. Eq. (42) expresses the Lagrangian corresponding to the objective (OBS$^{\text{DS}}$ defined in (1) (further specified by the expressions in Eq. (2)-(5)) with the addition of the constraints of Eq. (6)-(10), (23) and multiplied with their Lagrangian multipliers $(\gamma_t, \beta_t, \delta_t, \epsilon_t, \kappa_t)$.

$$\mathcal{L}_t^{\text{US}}[q_t^{\text{US}}, q_t^{\text{CC}_{\text{US}}}, q_t^{\text{CCS}_{\text{US}}}, q_t^{\text{CCU}_{\text{US}}}, q_t^{\text{CAP,CC}_{\text{US}}}, q_t^{\text{CAP,CONV}_{\text{US}}}, \gamma_t, \beta_t, \delta_t, \epsilon_t, \kappa_t] = -\text{OBJ}^{\text{US}} + \sum_1^t \tag{42}$$

$$\kappa_t(q_t^{\text{CC}_{\text{US}}} - q_t^{\text{CCU}_{\text{US}}} - q_t^{\text{CCS}_{\text{US}}}) + \gamma_t(q_t^{\text{US}} - q_t^{\text{CC}_{\text{US}}} - q_t^{\text{CONV}_{\text{US}}}) +$$

$$\epsilon_t(q_t^{\text{CC}_{\text{US}}} - q_t^{\text{CAP,CC}_{\text{US}}} - q_{t-1}^{\text{CAP,CC}_{\text{US}}} - \ldots - q_1^{\text{CAP,CC}_{\text{US}}}) +$$

$$\delta_t(q_t^{\text{CONV}_{\text{US}}} - (q_t^{\text{CAP,CONV}_{\text{US}}} - q_t^{\text{CAP,CC}_{\text{US}}}) - (q_{t-1}^{\text{CAP,CONV}_{\text{US}}} - q_{t-1}^{\text{CAP,CC}_{\text{US}}}) - \ldots - (q_1^{\text{CAP,CONV}_{\text{US}}} - q_1^{\text{CAP, CC}_{\text{US}}}) - q_0^{\text{CAP,CONV}_{\text{US}}})$$

The stationarity conditions in relation to the dual variables of Eq. (42) are given by Eq. (43)-(46):

$$\forall t : \kappa_t = \text{free} \quad \perp \quad \frac{\partial \mathcal{L}}{\partial \kappa_t} = \text{q}_t^{\text{CC}_{\text{US}}} = \text{q}_t^{\text{CCS}_{\text{US}}} + \text{q}_t^{\text{CCU}_{\text{US}}} \tag{43}$$

$$\forall t : \gamma_t = \text{free} \quad \perp \quad \frac{\partial \mathcal{L}}{\partial \gamma_t} = \text{q}_t^{\text{US}} = \text{q}_t^{\text{CC}_{\text{US}}} + \text{q}_t^{\text{CONV}_{\text{US}}} \tag{44}$$

$$\forall t : 0 \leq \delta_t \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial \delta_t} = \text{q}_t^{\text{TOT, CONV}_{\text{US}}} - \text{q}_t^{\text{CONV}_{\text{US}}} \tag{45}$$

$$\forall t : 0 \leq \epsilon_t \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial \epsilon_t} = \text{q}_t^{\text{TOT, CC}_{\text{US}}} - \text{q}_t^{\text{CC}_{\text{US}}} \tag{46}$$

The derivative of the Lagrangian to each of the primal variables leads to the formulation of six stationarity conditions in Eq. (47)-(52), each with the following orthogonal relationships:

$$\forall t: 0 \leq q_t^{\mathrm{CC_{US}}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\mathrm{CC_{US}}}} = -\mathrm{p}^{\mathrm{US}*} + \mathrm{E}^{\mathrm{CONV_{US}}}\mathrm{C}_t^{\mathrm{fuel_{US}}} + \mathrm{E}^{\mathrm{CC_{US}}}\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}})\mathrm{C}_t^{\mathrm{E}} + \mathcal{Z}^{\mathrm{ETS}_{I},\mathrm{US}}\alpha^{\mathrm{CC_{US}}}\chi^{\mathrm{CONV_{US}}}C_t^{\mathrm{ETS}}) + \epsilon_t + \kappa_t \tag{47}$$

$$\forall t: 0 \leq q_t^{\mathrm{CCS_{US}}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\mathrm{CCS_{DS}}}} = \chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}})(\mathrm{C}^{\mathrm{T}} + \mathrm{C}^{\mathrm{S}}) - \kappa_t \tag{48}$$

$$\begin{aligned}\forall t: 0 \leq q_t^{\mathrm{CCU_{US}}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\mathrm{CCU_{DS}}}} \quad &= \chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}})(\mathrm{C}^{\mathrm{T}}/2) + \mathcal{Z}^{\mathrm{ETS}^*_{I},\mathrm{US}}(1-\alpha^{\mathrm{CC_{US}}})\chi^{\mathrm{CONV_{US}}}\mathrm{C}_t^{\mathrm{ETS}_I} - \\ &\lambda_t^{\mathrm{CO_2}}\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}}) - \kappa_t\end{aligned} \tag{49}$$

$$\forall t: 0 \leq q_t^{\mathrm{CONV_{US}}} \quad \perp \quad 0 \leq -\mathrm{p}^{\mathrm{US}*} + \mathrm{E}^{\mathrm{CONV_{US}}}\mathrm{C}_t^{\mathrm{fuel_{US}}} + \mathcal{Z}^{\mathrm{ETS}_{I},\mathrm{US}}\chi^{\mathrm{CONV_{US}}}C_t^{\mathrm{ETS}} + \delta_t \tag{50}$$

$$\begin{aligned}\forall t: 0 \leq q_t^{\mathrm{CAP,CC_{US}}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\mathrm{CAP,CC_{US}}}} =& \frac{\mathrm{T}^{\mathrm{OPT}} - t + 1}{\mathrm{T}^{\mathrm{US}}}\mathrm{C}_t^{\mathrm{CAP,\ CC}}\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}}) - \epsilon_t - \epsilon_{t+1} - \ldots - \epsilon_T \\ &+ \delta_t + \delta_{t+1} + \ldots + \delta_T\end{aligned} \tag{51}$$

$$\forall t: 0 \leq q_t^{\mathrm{CAP,CONV_{US}}} \quad \perp \quad 0 \leq \frac{\partial \mathcal{L}}{\partial q_t^{\mathrm{CAP,CONV_{US}}}} = \frac{\mathrm{T}^{\mathrm{OPT}} - t + 1}{\mathrm{T}^{\mathrm{US}}}\mathrm{C}_t^{\mathrm{CAP,\ CONV}} - \delta_t - \delta_{t+1} - \ldots - \delta_T \tag{52}$$

From the above four equations, carbon capture will take place when the following expression holds (53), due to the orthogonality conditions:

$$\begin{aligned}\forall t: \kappa_t \leq &\Big(x_t^{\mathrm{CONV}}\mathrm{C}_t^{\mathrm{CAP,\ CONV}} - x_t^{\mathrm{CC}}(\mathrm{C}_t^{\mathrm{CAP,\ CONV}} + \mathrm{C}_t^{\mathrm{CAP,\ CC}}\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}}))\Big) + \\ &\Big(\mathrm{E}^{\mathrm{CONV_{US}}}\mathrm{C}_t^{\mathrm{fuel_{US}}} - (\mathrm{E}^{\mathrm{CONV_{US}}}\mathrm{C}_t^{\mathrm{fuel_{US}}} + \mathrm{E}^{\mathrm{CC_{US}}}\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}})\mathrm{C}_t^{\mathrm{E}})\Big) + \\ &\big(\mathcal{Z}^{\mathrm{ETS}_{I},\mathrm{US}}\chi^{\mathrm{CONV_{US}}}C_t^{\mathrm{ETS}} - \mathcal{Z}^{\mathrm{ETS}_{I},\mathrm{US}}\alpha^{\mathrm{CC_{US}}}\chi^{\mathrm{CONV_{US}}}C_t^{\mathrm{ETS}}\big)\end{aligned} \tag{53}$$

That means that κ_t should be smaller than the difference between fixed and variable cost of conventional production and production with carbon capture. The resulting lower bound, using equation (49) for $\lambda_t^{\mathrm{CO_2}}$ becomes (54).

$$\underline{\lambda_{\mathrm{t}}}^{\mathrm{CO_2}} = \overbrace{\frac{1}{\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}})}}^{\substack{\text{Normalised per}\\ \text{tCO2 captured per ton product}}} \left(\overbrace{\left(x_t^{\mathrm{CC}}(\mathrm{C}_t^{\mathrm{CAP,\,CONV}} + \mathrm{C}_t^{\mathrm{CAP,\,CC}}\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}})) - x_t^{\mathrm{CONV}}\mathrm{C}_t^{\mathrm{CAP,\,CONV}}\right)}^{\text{Difference in CAPEX for CCU and conventional production}} + \right. \tag{54}$$

$$\overbrace{\left((\mathrm{E}^{\mathrm{CONV_{US}}}\mathrm{C}_t^{\mathrm{fuel_{US}}} + \mathrm{E}^{\mathrm{CC_{US}}}\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}})\mathrm{C}_t^{\mathrm{E}} + \chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}})(\mathrm{C}^{\mathrm{T}}/2) - \mathrm{E}^{\mathrm{CONV_{US}}}\mathrm{C}_t^{\mathrm{fuel_{US}}}\right)}^{\text{Difference of OPEX for CCU and conventional production excluding carbon pricing}} +$$

$$\left. \overbrace{\left((\mathcal{Z}^{\mathrm{ETS}_{I,\mathrm{US}}}\alpha^{\mathrm{CC_{US}}}\chi^{\mathrm{CONV_{US}}}\mathrm{C}_t^{\mathrm{ETS}_I} + \mathcal{Z}^{\mathrm{ETS}^*_{I,\mathrm{US}}}(1-\alpha^{\mathrm{CC_{US}}})\chi^{\mathrm{CONV_{US}}}\mathrm{C}_t^{\mathrm{ETS}_I})) - \mathcal{Z}^{\mathrm{ETS}_{I,\mathrm{US}}}\chi^{\mathrm{CONV_{US}}}\mathrm{C}_t^{\mathrm{ETS}_I}\right)}^{\text{Difference of carbon pricing between CCU production and conventional production}} \right)$$

This expression signifies the difference between the variable and fixed costs of carbon utilisation and conventional production. Conventional capex disappears when legacy capacity is available. In the case that conventional production is rather inexpensive, carbon capture in combination with carbon utilisation can be made possible when a very high price for carbon is obtained. Carbon storage will not take place in this case as there are no revenues with this production route (and costs are assumed to be higher than conventional production in this scenario).

In case that carbon capture is less expensive than conventional production, the trade-off should be made between carbon utilisation and storage. If carbon utilisation takes place, the expression (55) holds, as derived from (48):

$$\kappa_t \leq (C_{\mathrm{T}} + C_{\mathrm{S}})\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}}) \tag{55}$$

With (49) a new lower bound for $\lambda_t^{\mathrm{CO_2}}$ can be obtained as expressed in (56) :

$$\underline{\lambda_{\mathrm{t}}}^{\mathrm{CO_2}} = \overbrace{\frac{1}{\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}})}}^{\substack{\text{Normalised per}\\ \text{tCO2 captured per ton product}}} \left(\overbrace{\left(\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}})(\mathrm{C}^{\mathrm{T}}/2) + \mathcal{Z}^{\mathrm{ETS}^*_{I,\mathrm{US}}}(1-\alpha^{\mathrm{CC_{US}}})\chi^{\mathrm{CONV_{US}}}\mathrm{C}_t^{\mathrm{ETS}_I}\right)}^{\text{OPEX for utilising carbon}} - \overbrace{(C_{\mathrm{T}} + C_{\mathrm{S}})\chi^{\mathrm{CONV_{US}}}(1-\alpha^{\mathrm{CC_{US}}})}^{\text{OPEX for storing carbon}} \right) \tag{56}$$

This expression signifies the difference between the variable costs of carbon utilisation and carbon storage.

C.3 Analytic understanding of ETS price fraction

The formula in Eq. (57) defines the threshold $\overline{\mathcal{F}}_{\text{ETS II/I}}$. A higher ETS fraction yields RFNBO production, while CCS (or conventional production) occurs below this threshold. Note, that $\overline{\mathcal{F}}_{\text{ETS II/I}}$ is time-dependent as it depends on the OPEX and CAPEX costs of the active bound upstream and the active bound downstream (with ETS II prices zero).

$$\overline{\mathcal{F}}_{\text{ETS II/I}}(t) = \frac{\mathrm{C}^{\text{ETS II}}(t)}{\mathrm{C}^{\text{ETS I}}(t)} = \frac{\text{Active Bound US(t) - Active Bound DS(t)}_{\text{ETS II = 0}}}{\mathrm{C}^{\text{ETS I}}(t)} \tag{57}$$

The bounds derived in Eq. (40), (41), (54) and (56), are further analysed in terms of the embedded ETS components. In

Fig. 7 those components are expressed using the ϵ-symbol to simplify the emissions multiplied with a certain ETS cost (C^{ETS}). The dynamic position of the bounds in relation to the ETS costs can be further analysed.

	Upstream lower bound	Downstream upper bounds
BOUND 1:	**CCU_{ETS} - CCS_{ETS} (active)**	**CCS_{ETS} - CU_{ETS} (active)**
Case 1 current regulation	**A.** $C^{ETS\ I}$	**C.** $(1/\varepsilon^{used})\varepsilon^{non\text{-}captured}C^{ETS\ I} + C^{ETS\ II}$
Case 2	**B.** 0	**D.** $(1/\varepsilon^{used})\ (\varepsilon^{non\text{-}captured}C^{ETS\ I} - \varepsilon^{RFNBO}C^{ETS\ I})$
BOUND 2:	**CCU_{ETS} - $CONV_{ETS}$ (alternative)**	**$CONV_{ETS}$ - CU_{ETS} (alternative)**
Case 1 current regulation	**E.** 0	**G.** $(1/\varepsilon^{used})\ \varepsilon^{all}\ C^{ETS\ I} + C^{ETS\ II}$
Case 2	**F.** $(1-\varepsilon^{all}/\varepsilon^{non\text{-}captured})C^{ETS\ I}$	**H.** $(1/\varepsilon^{used})\ (\varepsilon^{all}C^{ETS\ I} - \varepsilon^{RFNBO}C^{ETS\ I})$

Fig. 7: Indication of the emissions covered under each case study, each bound, both upstream and downstream.

Based on Fig. 7, the relative ETS fraction threshold $\overline{\mathcal{F}}_{\text{ETS II/I}}$ gets affected when the ETS I price increases. This can be derived from Eq. (58), obtained with bound A. and C. in Fig. 7. More intuitively, this equation shows that an increase in ETS I price requires a lower increase in the ETS II price to enable C(C)U.

$$\frac{\Delta C^{\text{ETS II}}}{\Delta C^{\text{ETS I}}} = 1 - \frac{\epsilon^{\text{DS}}_{\text{non-captured}}}{\epsilon^{\text{DS}}_{\text{used}}} \tag{58}$$

Consequently, a new threshold $\overline{\mathcal{F}}^{*}_{\text{ETS II/I}}$ could be defined based on the previous threshold $\overline{\mathcal{F}}_{\text{ETS II/I}}$ and ETS I price.

$$\overline{\mathcal{F}}^{*}_{\text{ETS II/I}} = \frac{C^{\text{ETS II}*}}{C^{\text{ETS I}*}} = \frac{\Delta C^{\text{ETS I}}(1 - \frac{\epsilon^{\text{DS}}_{\text{non-captured}}}{\epsilon^{\text{DS}}_{\text{used}}}) + C^{\text{ETS I}}\overline{\mathcal{F}}_{\text{ETS II/I}}}{C^{\text{ETS I}*}} \tag{59}$$

Appendix D
Auxiliary results

D.1 Auxilary results on bounds sensitivity

To capture the parameter variability on the bounds position and production outcomes Fig. 8 has been created. This tornado-like diagram shows on the vertical axis the parameters that are evaluated relative to the base run using half (left of the horizontal axis) or twice (right of the horizontal axis) the parameter value from the base run. Hence, the base run parameters serve as a reference for which no high or low parameter change is applied, while for all the other runs only one parameter has been changed at the time to either a low (x0.5) or higher (x2) value. The horizontal axis shows the relative fractional change of the total average production under each parameter to the base run for both the upstream industry (top, darker bars) and the downstream industry (bottom, lighter bars). No time-relation has been shown in this figure as all values are averaged over the entire time span.

An ETS II over I fraction of 0.7 has been applied due to the close proximity of the lower and upper bounds in Case 1. As such, changes in parameters will readily result in investment changes when the upper or lower bound is shifted up or downwards. As discussed earlier, the ETS II over I fraction does not influence the bounds in Case 2 leading to very similar outcomes when another ETS fraction is picked.

Fig. 8 shows that with an ETS fraction of 0.7 RFNBO production will take place for less than 10% of the total average production in the base run of Case 1. Time-based analysis indicates that this occurs from the year 2049 onward. Lower values in electricity and energy requirements for RFNBO production can advance the RFNBO production in Case 1, while lower emissions of crude oil production will eliminate C(C)U. These are intuitive outcomes. Besides, a higher storage price will negatively affect the amount of CCS.

It also becomes apparent that an increase in ETS I price will stimulate more CCS in Case 1. It can be explained by the parameter $\mathcal{F}_{\text{ETS II/I}}$ that reduces by half when only ETS I increases. Higher ETS I prices increase the surrendering burden upstream, while ETS II does not provide a sufficient incentive to produce RFNBOs. Lower ETS I prices will initially prolong the conventional phase, but also reduce the surrendering burden enabling RFNBO production afterwards. To maintain the ETS fraction of 0.7, both ETSs are changed. By increasing both ETSs prices, RFNBO production takes place. This shows us that under higher ETS prices, the CCS-C(C)U trade-off will indeed occur at a slightly lower ETS fraction compared to the base run. Instead of a fraction of 0.68, a fraction of 0.58 is perceived in this case. Eq. (59) confirms that number, where $\overline{\mathcal{F}}^*_{\text{ETS II/I}} = \frac{150\times0.472+150\times0.678}{300} = 0.58$.

In Case 2 with primarily CCU production during the base run, the four parameters: ETS price, electricity price, energy for RFNBO and emissions of crude oil, are also predominantly affecting the production outcome. A higher electricity price results indeed in CCS indicating that the upper bound has shifted below the lower bound. The CAPEX of the RFNBO installation can also affect and delay the CCU uptake when the cost doubles.

In contrast to Case 1, variations in ETSs prices are more intuitive in Case 2. A decrease in those prices will decrease RFNBO production and stimulate more conventional production. As the ETS II over I fraction does not play a role in Case 2, a drop in ETS II will only cause a bit more production downstream, the production choices do not change.

The effect of all other parameters (energy for carbon capture, size of upstream compared to downstream firm and cost of storage) hardly affects the production results for both cases. Besides, note that with an ETS fraction equal to 1 (i.e. ETS I equal to ETS II), the diagrams of Case 1 and Case 2 look almost identical, equal to the current diagram of Case 2 in Fig. 8. Only the ETS I effect will change the solution of Case 1 compared to Case 2, but that has to do with the fraction that changes, only influencing Case 1. Again, this confirms that the same solution is obtained under equal ETSs.

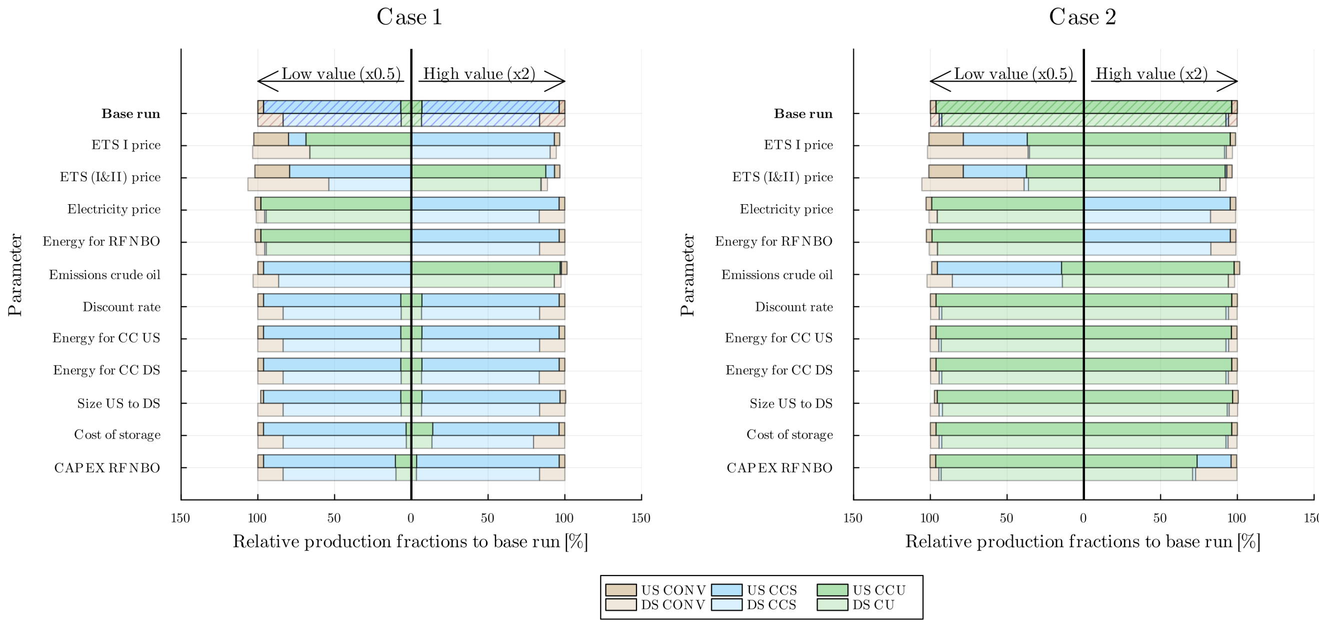

Fig. 8: Sensitivity analysis in a tornado-like diagram expressing the effect of low and high parameter values on production fractions relative to the base scenario/run for both Case 1 and Case 2. This diagram has been made for an ETS II over I fraction equal to 0.7 and an ETS I price equal to 150 €/tCO_2.

D.2 Auxilary results welfare vs. emissions abated

Fig. 9 contains the split welfare between the three markets (upstream, downstream and ETS). The outer left plot corresponds to Fig. 6. Note that costs upstream and downstream are now including ETS expenses. Adding both market results and subtracting those ETS expenses yields the left plot indicating the joint market outcome equal to Fig. 6. We can deduce that higher ETS expenses in Case 1 are related to high carbon-intensive refinery activities downstream in contrast to the carbon utilisation route as obtained for all ETS scenarios in Case 2. No remarkable differences in welfare distributions between both cases in upstream and downstream markets are perceived. A higher ETS II price downstream leads to higher economic losses. The influence of a higher ETS II price upstream is negligible as it is only indirectly affected by downstream CO_2 demand in the case that CO_2 commodity trading takes place.

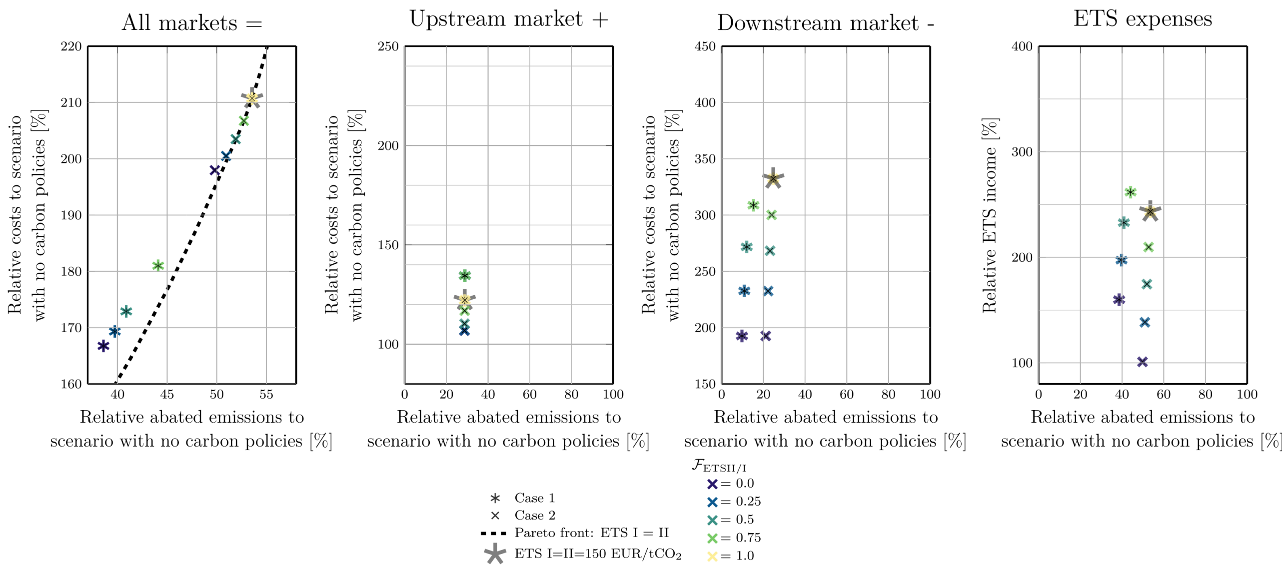

Fig. 9: Relative costs including welfare losses due to demand reduction and emissions in relation to the scenario with no carbon policies. The four subplots are related to the joint market, the upstream market, the downstream market and the ETS market respectively.

Note that in order to qualify as an RFNBO product, the emissions compared to the conventional production route should be reduced by 70%. This excludes product-use emissions till 2040 if the captured CO_2 is derived from fossil industries, after that those product-use emissions become part of the emission reduction calculation as well. However, it does include energy-related emissions. Consequently, for this case study, the allowed carbon intensity of electricity production should be lower than 24 g CO_2 per kWh until 2040 and is applied to all markers. This is roughly 1/8 of the current average European power sector's emission intensity [45]. After 2040 it is only possible to qualify as a (carbon-contained) RFNBO product with negative emissions technologies, i.e. biogenic or atmospheric captured CO_2.

Applying a higher carbon intensity to electricity production will result in an increased carbon footprint of C(C)U relative to that of CCS due to a larger energy dependence. If this is properly reflected by an increase in the electricity price, both Case 1 and Case 2 will yield the exact same solution i.e. CCS production will dominate for all years and all ETS fractions. This result is obtained with Fig. 10. The shift to CCS is characterised by a shift of the downstream bounds due to the higher electricity cost, decreasing its willingness to pay for CO_2 commodity. The CCS lock-in in Case 1 will disappear as CCS becomes the most cost-effective emission abatement technology represented by the modelling framework. The remaining gap between the case's markers and the Pareto front is now purely related to non-harmonised ETS prices. As a consequence, prioritizing low-emission power generation e.g. as is done in the form of the RFNBO definition and related quotas, is key to making sure that enough emission abatement efforts can be realised, effectively decarbonising the refinery industry.

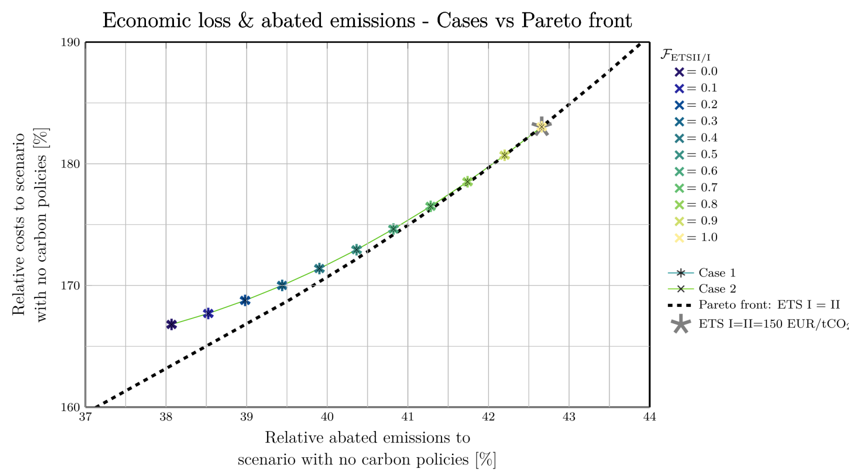

Fig. 10: Economic loss in relation to the abated emissions with high electricity carbon intensity levels.