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CO_2 storage or utilization? A real options analysis under market and technological uncertainty

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Abstract

Carbon Capture and Storage (CCS) and Carbon Capture and Utilization (CCU) are considered essential solutions to reduce greenhouse gas (GHG) emissions worldwide. A crucial difference between the two is that CCS is already a mature technology, while CCU is still in the R&D phase. Hence, firms are confronted with a dilemma, where they have to choose between either the mature CCS, the emerging CCU, or the installation of both in a Carbon Capture Utilization and Storage (CCUS) system. In this study, we analyze different strategies that the firm can pursue and determine the optimal investment timing. In doing so, we take into account both technological uncertainty, i.e. the unknown time-to-market of CCU, and market uncertainty, i.e. the CO_2 price. Three different CCUS value chains in the cement industry are analyzed. We find that the anticipated arrival of profitable CCU technologies in the future does not delay investments in CCS in the current period. Investments in CCS and CCU can be accelerated by reducing the volatility of the CO_2 price, or by increasing the growth rate of the CO_2 price. Finally, we find that a higher fraction of CO_2 emissions that can be used in CCU, results in sooner adoption of CCS today.

Keywords— Carbon Capture and Utilization, Carbon Capture Utilization and Storage, Real Options Analysis, Dynamic Programming, Technological Innovation

1 Introduction

Despite the growing sense of urgency to tackle climate change, the CO_2 emission levels still rose by 6% in 2021. This is in stark contrast with the ambitious goals from the European Union, which has expressed the ambitions to emit 55 % less greenhouse gas (GHG) emissions by 2030, compared to 1990, and to become the first climate-neutral continent by 2050 (EC, 2022). Besides investments in renewables, increased energy efficiency, and alternative transport modes, the EU's long-term vision to become climate-neutral by 2050 also includes Carbon Capture and Storage (CCS) to abate the remaining CO_2 emissions (EC, 2018). CCS captures, transports, and finally stores the CO_2 permanently underground, either on- or offshore. In addition to CCS, the European Commission also recognizes a role for Carbon Capture and Utilization (CCU) in the pathway to climate neutrality (EC, 2021). CCU uses the captured CO_2 as a valuable commodity and transforms it into marketable products (e.g. fuels, chemicals, building materials), which generates additional revenues. Finally, both technologies can also be integrated into a Carbon Capture Utilization and Storage (CCUS) value chain.

CCS and CCU are expected to play an important role in the transition to a climate-neutral society, as illustrated by their recognition as key technologies for reaching climate targets in the latest report of the Intergovernmental Panel on Climate Change (IPCC) (IEF, 2022). Despite their central role in many mitigation strategies, the deployment of CCS and CCU remains too slow. CCS projects are delayed because of their high costs, a lack of public acceptance, and clear policy support (Bui et al., 2018). CCU is lagging even further in terms of deployment. Most CCU technologies are not yet ready to be commercialized, and their expansion to a commercial scale would require high volumes of renewable energy and green hydrogen in the future (EC, 2023a). In sum, various economic, technical, and societal barriers currently hamper the deployment of CCS and CCU.

To solve some of these barriers and further support the deployment of CCS and CCU technologies, the European Commission has established different policy initiatives. For example, the CCS Directive provides a legal framework to guarantee the safe storage of CO_2 and the Renewable Energy Directive includes incentives to increase the production of fuels by CCU. In 2005, the EU launched the world's very first Emissions Trading System (ETS), allowing the trade of emission allowances between various countries. In May 2023, the EU ETS regulations were revised to mirror the ambitious climate targets of the EU. Under the current EU ETS directive, the obligation to surrender emission allowances is lifted for CO_2 emissions that are captured and transported for permanent storage (Article 12(3a)), and for CO_2 emissions that have been utilised in such a way that they are permanently chemically bound (Article 12(3b)) (EC, 2023b).

The novelty of CCS and CCU, the possibility of combining CCS and CCU, and the emerging policy support add to the complexity of the decision to invest in CCS, CCU, or CCUS projects. Previous studies have analyzed these investment decisions in multiple ways. A large body of literature assesses the profitability of novel CCS or CCU solutions, typically by performing techno-economic assessments (TEAs) (see Lamberts-Van Assche and Compernolle (2022a) for a review of economic feasibility studies for CCU projects). One common concern in all studies is the high level of uncertainty about the future performance of CCS and CCU projects. However, TEA studies typically only consider the investment decision in a deterministic setting and hence, can only advise to either adopt the technology now, if it is profitable, or never, if it is too costly. The uncertainties and risks of the real-world setting are typically neglected in this type of assessment. To include those uncertainties and risks, there is a growing stream of literature that analyzes investment decisions in CCS or CCU technologies in a dynamic framework, taking managerial flexibility into account (see Agaton (2021) and Lamberts-Van Assche and Compernolle (2022b) for an extensive review of real options applications in CCS and CCU respectively). Real options analysis presents a method to value flexibility in investment decisions, acknowledging the fact that decision-makers can delay investment decisions in practice (Dixit and Pindyck, 1994). A literature review on real options analysis for CCU projects revealed that the CO_2 price is the most commonly included source of uncertainty in investment decisions for CCU projects (Lamberts-Van Assche and Compernolle, 2022b). The CO_2 price in the EU ETS can also be affected by policymakers, by changing the emissions cap and the number of emissions allowances issued. Despite the growing number of studies on investments in CCS and CCU projects, the existing literature does not yet address all the complexities associated with these investment decisions.

First, CCS and CCU should not only be considered as two stand-alone solutions but also as technologies that are compatible and can be integrated into one CCUS installation. To avoid a mismatch between the scale of the CO_2-emitting plant, on the one hand, and the scale of the CO_2 utilization plant, on the other hand, a CCUS value chain is created (Monteiro and Roussanaly, 2022). Hence, the possibility of combining CCS and CCU is included in our real options model.

Second, CCS and CCU are at different levels of maturity. While CCS has reached the highest Technology Readiness Level (TRL) of 9 and large-scale CCS projects exist, CCU technologies are mostly still at the lab or prototype scale (TRL 4-5) (Bui et al., 2018). This discrepancy in maturity confronts firms with a complex decision problem. The firm can start reducing its CO_2 emissions immediately, by investing in CCS today. Alternatively, the firm can wait for CCU to mature, keeping the option open to adopt the technology that is expected to be more profitable. In other words, the firm needs to anticipate the arrival of more profitable technologies (i.e. CCU) in the future, while making investment decisions for existing technologies (i.e. CCS) today. Although real options studies have included the effect of technological progress on investments in CCU projects before, these studies did not consider decisions in technologies with different levels of maturity. The majority of these studies use learning curve models to describe the technological progress, assuming a continuous decline in the costs (Lin and Tan, 2021; Zhang et al., 2014; Yang et al., 2019; Zhang et al., 2021). Deeney et al. (2021), however, model the technological innovation in a CCU project by a Poisson process, to mimic sudden breakthroughs. In our real options model, the Poisson process is used to simulate the market entrance of CCU.

These two complexities - the possibility to invest in CCS and CCU separately, as well as jointly, and their difference in technological maturity - have so far not been addressed in the literature. This study fills this gap by analyzing the decision to invest in a CCS, CCU or CCUS value chain, in a dynamic framework that allows the potential investor to have some flexibility in the timing of the investment. Therefore, this study develops a real options model that allows for choosing between these technologies with different levels of technological maturity or combining them in a CCUS value chain. The real options models will help decision-makers to calculate the CO_2 price level that should be surpassed in the EU ETS before it is optimal to invest in either CCS, CCU or CCUS. Two uncertainties are included in the model: technological uncertainty, i.e. the unknown time-to-market of CCU, and market uncertainty, i.e. the unknown future evolution of the CO_2 price. The real options model is then applied to potential CCUS chains in the cement industry, which is responsible for 6 to 7% of global CO_2 emissions (Monteiro and Roussanaly, 2022). About two-thirds of these CO_2 emissions are unavoidable, highlighting the need for CCUS to reduce CO_2 emissions in the cement industry (IEA, 2019).

Applying our framework to the cement industry results in the following findings. We find that a higher volatility in the CO_2 price, i.e. more market uncertainty, delays the investment in both CCS and CCU. The results also indicate that firms will not necessarily postpone their investment in CCS, because they anticipate the arrival of a more profitable CCU technology in the future. On the contrary, we even observe slightly lowered CO_2 price thresholds to invest in CCS, when more attractive CCU solutions are expected in future periods. However, how soon the arrival of CCU is expected, does not affect the investment threshold to a large extent.

Our main contributions can be summarized as follows. First, this study adds to the existing literature by recognizing the complementary nature of CCU and CCS and showing how this affects the investment decision in both CCU and CCS individually and CCUS jointly. Second, this study demonstrates how firms that consider the flexibility in the timing of the investment and the technological and market uncertainties, will delay their investment in CCS and CCU. This is the optimal decision for a firm considering their economic interest, but it may not be the most desirable decision from a societal perspective. Third, and adjacent to the previous finding, policymakers should guarantee more predictability and a higher growth rate in the CO_2 price in the EU ETS, if they want to minimize the delay in CCUS investments. Finally, this study reveals that the anticipation of a more attractive CCU solution in the future does not delay the investment in CCS today This means that CCU and CCS technologies do not necessarily have to be seen as two competitive pathways to reduce CO_2 emissions.

The remainder of the article is organized as follows. Section 2 presents the set-up of the four real options models, one for each possible investment strategy. Section 3 presents the results of the real options models, for three CCUS value chains in the cement industry. In Section 4, we analyze how the investment thresholds shift in response to changes in certain parameters of the model, e.g. the arrival rate of CCU and the volatility in the CO_2 price. Our conclusions are given in Section 5.

2 The model setup

We consider a risk-neutral, profit-maximizing firm that emits CO_2 and needs to surrender emission allowances under the EU ETS. Possible solutions to reduce its CO_2 emissions, and the associated purchases of emissions allowances, are the mature CCS, the emerging CCU, or a combination of both. To reduce its CO_2 emissions and the associated emission allowances that need to be bought, the firm is considering an investment in CCS, CCU, or CCUS. We propose a dynamic framework to find the firm's optimal strategy to reduce its payments in the EU ETS, under both technological (the unknown time-to-market of CCU) and market uncertainty (the CO_2 price). This framework is built using a real options approach, that acknowledges the flexibility in the firm's investment decisions and includes the present uncertainties. This setup is similar to the well-cited work of Grenadier and Weiss (1997), which develops a real options model to find the optimal investment decision for a firm confronted with a sequence of innovations and identifies four different adoption strategies. In the current study, the sequence of innovations is presented by CCS (the existing technology) and CCU (the future innovation). The present study provides the first framework to acknowledge that the existing and future innovations are not necessarily mutually exclusive, but can also be combined. This study assumes that the firm optimizes its investment decisions over an infinite time horizon, where time is continuous.

The unknown arrival of CCU in the future is a source of technological uncertainty. We consider a firm that does not influence or accelerate the arrival of CCU by investing in R&D: the R&D process is exogenous to the firm. We model the firm's perceived probability of CCU arriving in the next period by a Poisson jump process. Due to the R&D nature of CCU projects, the discrete jumps of a Poisson process are fit to describe breakthroughs in the CCU project (Deeney et al., 2021). A Poisson process with intensity λ means that the probability of CCU maturing in the next period equals λdt.

The CO_2 price in the EU ETS presents a source of market uncertainty. The carbon price level is driven by various forces, including policy measures, commodity prices or geopolitical events. We assume that the CO_2 price evolution follows a Geometric Brownian Motion (GBM) (see e.g. Abadie et al., 2014; Compernolle et al., 2017; Compernolle and Thijssen, 2022; Zhang et al., 2014) and is described as follows

$$dE = \alpha E dt + \sigma E dz, \tag{1}$$

with E the price for an emission allowance per tonne of CO_2 in the EU ETS, or simply the CO_2 price, α the drift or growth rate, σ the variance or volatility, and dz the increment of a Wiener process. In the real options model, the CO_2 price is included as a revenue per ton of CO_2 stored or utilized: the assumption is that both the stored CO_2 and the utilized CO_2 are considered as not-emitted in the EU ETS and consequently, no allowances need to be surrendered anymore for the stored or utilized CO_2. In practice, not all utilized CO_2 is considered not-emitted in the EU ETS. As mentioned earlier, the obligation to surrender emission allowances in the EU ETS is lifted for CO_2 emissions that are captured and then (1) transported for permanent storage or (2) that have been utilised in such a way that they are permanently chemically bound (EC, 2023b). Hence, the present study includes an optimistic scenario where utilized CO_2 is always considered as not-emitted in the EU ETS, independent of the utilization route.

For the profit-maximizing firm, it will only be optimal to invest in emission abatement projects when the CO_2 price is high enough, resulting in higher cost savings. The investment decision in CCS, CCU or CCUS will be triggered by threshold CO_2 prices, which we denote by E^*_{ccs}, E^*_{ccu} and E^*_{ccus}, at which the firm is indifferent between waiting or investing in CCS, CCU and CCUS respectively. To determine the optimal investment time, the first step is to identify the optimal strategy when CCU is mature and ready to install. Once we have determined the conditions under which each adoption strategy is optimal in the presence of CCU, we can start analyzing what happens before CCU arrives. Therefore, the real options model to analyze the investment strategy is split into two stages: one before and one after the arrival of the CCU technology. To identify the variety of technology adoption strategies that are possible over the course of both stages, we need to understand the features of each abatement technology first.

If the firm adopts CCS, all of its CO_2 emissions are captured and stored permanently underground.[1] To put CCS into operation, the firm needs to pay a one-time investment cost for the capture facility, a capture cost per tonne of CO_2 and a transport and storage fee to a third party. In other words, the transport and storage of the CO_2 is 'outsourced': a fee is paid per ton of CO_2 to a firm specialized in the transport of CO_2 to a site where the CO_2 can be stored permanently. An example of a potential partner for the transport and storage of CO_2 is the Longship project, which will be the first cross-border transport and storage infrastructure network, offering the underground storage of CO_2 in Norway.

With CCU, the CO_2 is not stored underground, but converted into valuable products. Because the amount of CO_2 that can be utilized is limited - both due to market and technical limitations - not all CO_2 emissions of the firm will be captured and converted in the CCU value chain (Markewitz et al., 2012). Hence, if the firm adopts only the CCU technology, the firm will still need to buy emission allowances for the remaining CO_2 emissions. To adopt CCU, the firm needs to incur sunk investment costs for the capture facility and the utilization plant and needs to pay a capture cost and utilization cost per tonne of CO_2 used. In contrast to CCS, the firm will now receive revenues, from the sales of the products resulting from the conversion of CO_2.

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[1] In the literature, the assumption of a 90% capture rate has become standard. However, capture rates will need to go beyond 90%, to reach climate targets. Capture rates up to 98% are feasible at relatively low marginal costs (Brandl et al., 2021). In this study, we assume that 100% of the CO_2 can be captured and stored.

Finally, the CCUS pathway combines both CCS and CCU. The part of the CO_2 emissions that can be used and converted are sent to the utilization plant on-site. The remaining part of the CO_2 emissions is transported to the storage site to be stored underground. Hence, all CO_2 emissions are avoided. The firm needs to pay investment costs for both the capture facility and the utilization plant, and needs to pay capture costs for all CO_2, the transport and storage fee for the part that is stored and the utilization cost for the fraction of CO_2 emissions that is used.

From these costs it follows that one of the assumptions of the real options model is that the same firm, or the same decision-maker, can invest in (1) the capture facility, to capture the CO_2, and (2) the utilization plant, in which the CO_2 is used and converted into other valuable products. Examples of future CCUS value chains, where one actor both invests in the CO_2 capture and the CO_2 utilization technology, could be imagined for many different types of industries. For example, a chemical plant could invest in a CCU-route that utilizes the CO_2 from its flue gases to produce methanol, or a cement plant could utilize the CO_2 to produce CCU-based building materials. The assumptions that are made for each abatement technology in this study are summarized in Table 1. Figure 1 visualizes the value chain for each abatement technology, highlighting both the differences and similarities between the three pathways.

Considering the assumed parameters for each technology (Table 1) and the two-staged nature of the investment problem, six possible technology adoption strategies can be identified. In Stage 1, the firm has only two options: invest in CCS, or wait. If the firm adopted CCS in Stage 1, the firm can hold on to CCS (1) or adopt CCU in Stage 2 (2), to reach the hybrid CCUS solution. If the firm waited in Stage 1, the firm can still decide to invest in CCS alone (3), invest in CCUS simultaneously (4), adopt CCU and CCS in a sequential order (5) or invest in CCU immediately when it arrives (6) in Stage 2.

Figure 2 summarizes the various technology adoption strategies that are possible over both stages.

	CCS	**CCU**	**CCUS**
Goal	CO_2 storage	CO_2 utilization	CO_2 storage & utilization
Emission allowances	0	> 0	0
Investments	Capture facility	Capture facility Utilization plant	Capture facility Utilization plant
Variable costs	Capture costs Transport & storage fee	Capture costs Utilization costs	Capture costs Transport & storage fee Utilization costs
Revenues		CO_2-based product	CO_2-based product

Table 1: Comparison of the three abatement technologies: CCS vs. CCU vs. CCUS.

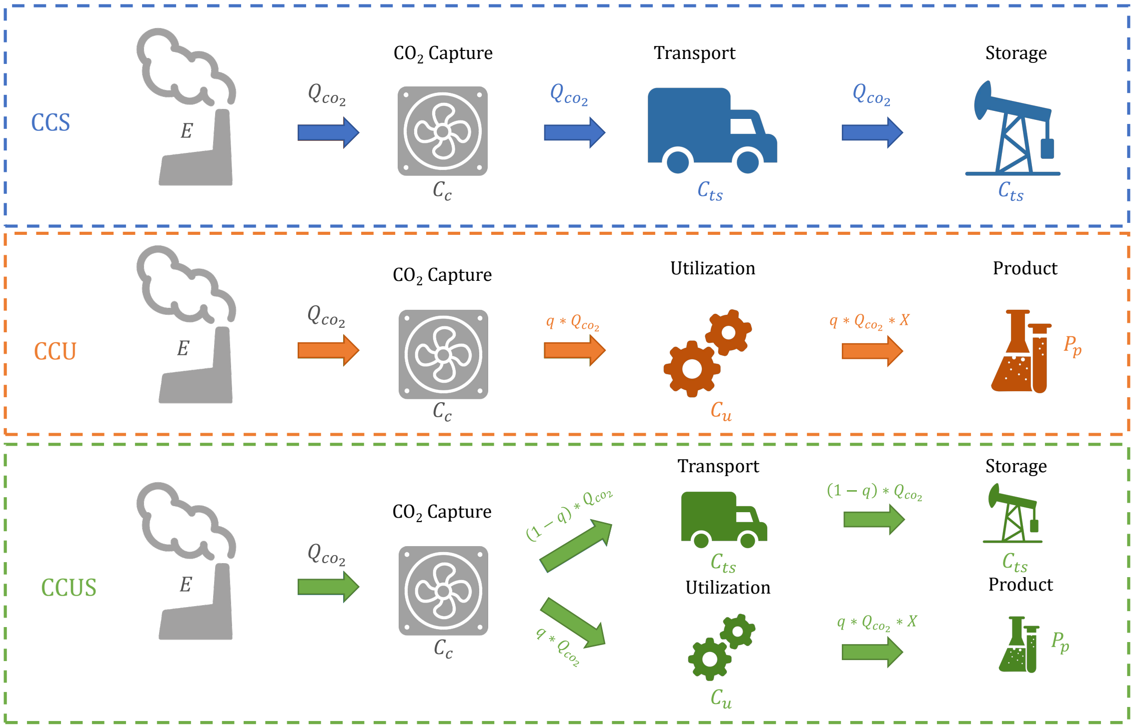

Figure 1: The value chains for CCS, CCU and CCUS.

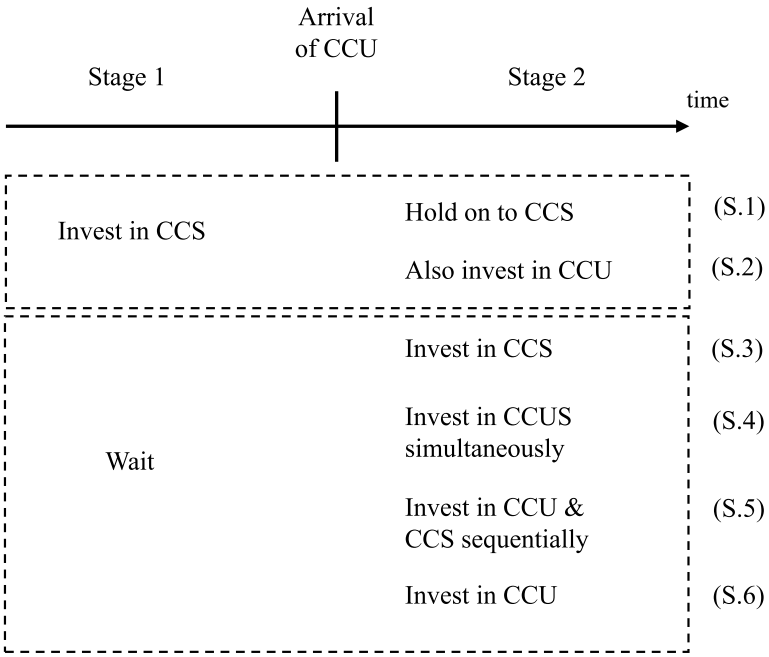

Figure 2: Six technology adoption strategies over Stages 1 and 2.

To determine the optimal decision in Stage 1 (wait or invest in CCS), the firm needs to understand the consequences of its decision today on its future opportunities. If the firm invests in CCS in Stage 1, it can hold on to CCS or invest in CCU as well in Stage 2. Only if CCUS results in a higher project value than CCS, the firm should also invest in CCU in Stage 2. If, however, the firm waited in Stage 1, more adoption strategies still remain open, as summed up in Figure 2.

A comparison of the project values of CCS, CCU and CCUS enables us to identify the optimal adoption strategy in Stage 2, after waiting in Stage 1. The present value V of each abatement technology over an infinite time horizon, taking into account the expected growth rate α in the CO_2 price E, is expressed as follows

$$V_{ccs} = \frac{Q_{co_2}}{\rho - \alpha} \cdot E - \frac{Q_{co_2}}{\rho} \cdot (C_c + C_{ts}) - I_c, \tag{2}$$

$$V_{ccu} = \frac{q \cdot Q_{co_2}}{\rho - \alpha} \cdot E + \frac{q \cdot Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_c - C_u) - I_c - I_u, \tag{3}$$

$$V_{ccus} = \frac{Q_{co_2}}{\rho - \alpha} E - \frac{Q}{\rho} \cdot C_c - \frac{(1-q) \cdot Q_{co_2}}{\rho} \cdot C_{ts} + \frac{q \cdot Q}{\rho} (P_p \cdot X - C_u) - I_c - I_u, \tag{4}$$

where ρ represents the discount rate (with $\rho > \alpha$ [2]), Q_{co_2} represents the amount of CO_2 emissions from the firm, C_c the capture cost per tonne of CO_2, C_{ts} the transport and storage fee per tonne of CO_2, q the fraction of the CO_2 emissions that can be utilized, P_p the price for the CO_2-based product, X the conversion factor from CO_2 to the product and C_u the utilization cost per tonne of CO_2. The investment costs for the capture and utilization plant are respectively I_c and I_u.

Figure 3 plots the present values of the cash flows that are generated by CCS, CCU and CCUS as a function of the CO2 price. The present values of each technology (CCS, CCU or CCUS) are ranked relative to each other in four different scenarios, when it is optimal for the firm to (a) invest in CCS alone, (b) invest in CCS and CCU simultaneously, (c) adopt CCU and CCS sequentially, at different CO2 prices, and (d) invest in CCU immediately. These scenarios reflect the adoption strategies (S.3) – (S.6) that were presented in Figure 2, where the firm waits in Stage 1 until CCU arrives. If the firm invests in CCS in Stage 1, the present value of CCU alone (red line) is no longer relevant. Figure 3 (a) then represents the scenario where the firm should hold on to CCS (S.1). Figures 3 (b) – (d) present scenarios where the firm should also invest in CCU (S.2) since the present value of CCUS is higher than the present value of CCS.

Based on Figure 3, we can derive the conditions under which each of these strategies is optimal. We do so by comparing the investment cost for the utilization plant I_u to the net benefits of CCU, denoted by F. These net benefits represent the cashflows that are generated by operating CCU, in addition to CCS. Hence, F equals the revenues for the CO_2-based product ($P_p \cdot X$), plus the avoided transport and storage costs (C_{ts}), minus the utilization costs (C_u).

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[2] The assumption $\rho > \alpha$ guarantees that all present values are finite.

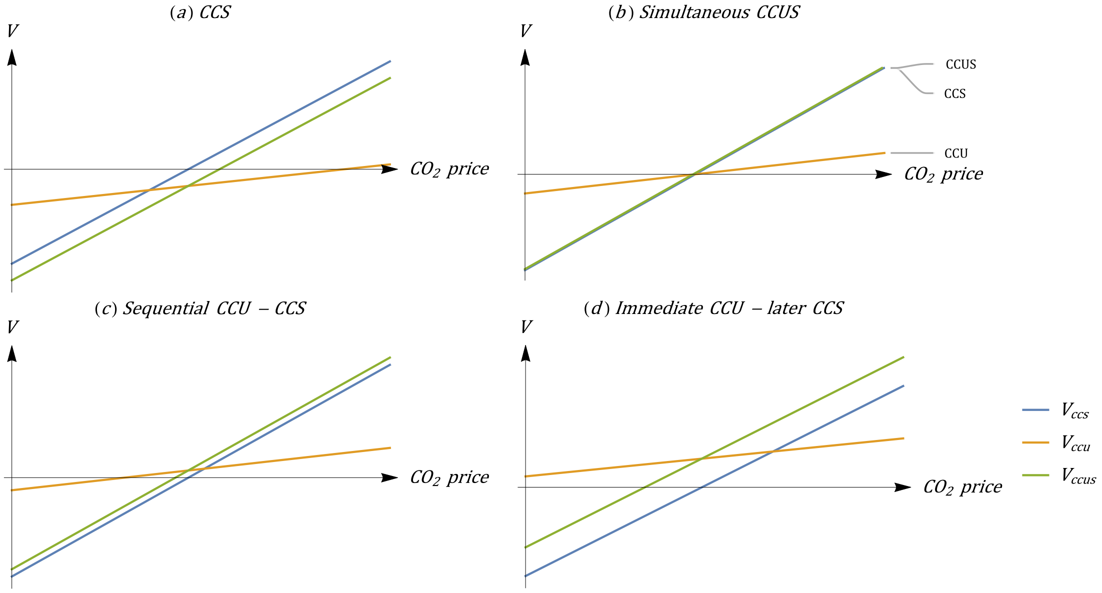


Figure 3: The present values of CCS, CCU and CCUS in Stage 2 for different scenarios where the optimal adoption strategy is to (a) invest in CCS alone, (b) invest in CCUS simultaneously, (c) invest in CCU and CCS sequentially, or (d) invest in CCU immediately and in CCS later, after the firm waited in Stage 1.

Figure 4 plots the investment cost for the utilization plant I_u against the net cashflows N from operating CCU, to draw the four optimal regions and their boundary conditions. When the investment cost I_u for the utilization plant is high and the net CCU cashflows N are low, the optimal adoption strategy for the firm is to invest in CCS alone (red). When the investment cost decreases or the net benefits of CCU increase slightly, it is optimal for the firm to invest in CCUS simultaneously (dark purple). At further declining I_u or increasing N, the attractiveness of CCU rises. In the light purple area, the firm will invest sequentially in CCU and CCS: first in CCU alone, and later, at high enough CO_2 prices, also in CCS. Finally, as I_u becomes lower and N continues to rise, the firm will invest in CCU immediately when it arrives (independent of the CO_2 price) and later invest in CCS (blue). Similar to Figure 3, the regions (a) - (d) reflect the optimal adoption strategies (S.3)-(S.6) from Figure 2. However, we can also observe the optimal regions for adoption strategies (S.1)-(S.2) in Figure 4. In region (a) (red area), the firm should hold on to CCS, whereas in regions (b)-(d) (purple and blue areas), the firm should also invest in CCU.

Whether the firm already invested in CCS in Stage 1 or is still waiting when CCU enters the market will depend on the arrival time of CCU and the profitability of both CCS and CCU. To model these dynamics, a real options approach is necessary. In the next sections, we perform a rigorous real options analysis to identify the CO_2 price thresholds for each abatement technology in both stages, $E^*_{ccs,1}$,$E^*_{ccu,2}$, $E^*_{ccs,2}$ or $E^*_{ccus,2}$. These investment thresholds are not simply the break-even points of the present value curves in Figure 3, but also take into account the value of flexibility due to the uncertainty in the CO2 price. As a result, these ‘real options’ investment thresholds can either be lower or higher than the traditional investment thresholds. Because the optimal adoption strategy and required investment thresholds are different in each region from Figure 4, the real options models are developed separately for each region in the following sections.

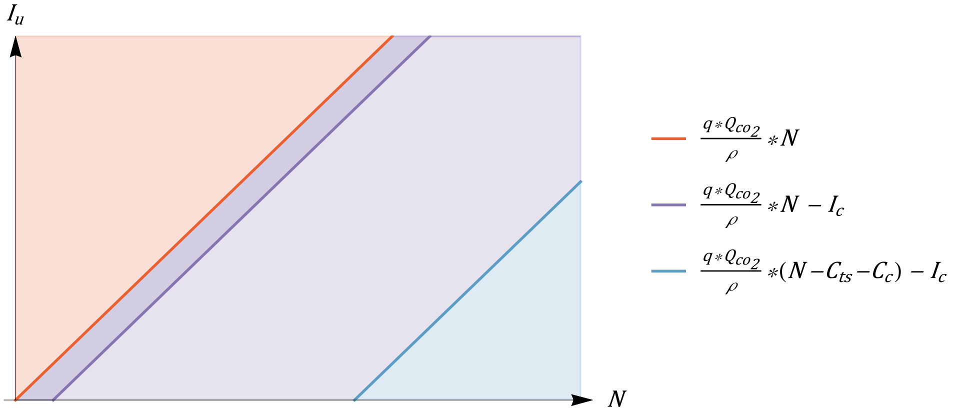


Figure 4: Four optimal regions for each adoption strategy in Stage 2, defined by investment I_u and net benefits N of CCU: (a) CCS (red); (b) simultaneous CCUS (dark purple); (c) sequential CCU - CCS investment (light purple); (d) immediate CCU investment, followed by CCS (blue), after the firm waited in Stage 1.

2.1 Model 1: CCS

In Model 1, we analyze the optimal investment timing for the red region in Figure 4, where CCS yields the highest return for the firm. As shown in Figure 3, CCS can reach break-even at the lowest CO_2 price and always returns the highest value afterwards. To find the optimal timing to invest in CCS, the firm needs to determine the CO_2 price threshold E^*_{ccs}. Using the dynamic programming technique, as described in Dixit and Pindyck (1994), we can solve this investment decision problem and find the threshold E^*_{ccs}. Model 1 describes how to find the optimal timing to invest in CCS, either in Stage 1 (before CCU arrives) or in Stage 2 (after CCU arrives). Hence, Model 1 develops the adoption strategies (S.1) and (S.3) from Figure 2.

When $E > E^*_{ccs}$, it is optimal to invest in CCS and the firm obtains the project value V_{ccs} (2):

$$F_1(E) = \frac{Q_{co_2}}{\rho - \alpha} \cdot E - \frac{Q_{co_2}}{\rho} \cdot (C_c + C_{ts}) - I_c. \tag{5}$$

As long as $E \leq E^*_{ccs}$, it is optimal for the firm to wait with the investment and hold on to the option to invest in CCS. The first step to find this option value, is the preparation of the Bellman equation (Dixit and Pindyck, 1994):

$$\rho \cdot F_1(E) = \lim_{dt \to 0} \frac{1}{dt} \cdot \mathbb{E}[dF_1]. \tag{6}$$

The second step is to apply Ito's Lemma, which is used to determine $\mathbb{E}[dF]$. The Bellman equation in (6) is expanded using Ito's Lemma, resulting in the Ordinary Differential Equation (ODE):

$$\frac{1}{2}\sigma^2 E^2 F_1^{''}(E) + \alpha E F_1^{'}(E) - \rho F_1(E) = 0. \tag{7}$$

The solution of (7) is given by 8, which reflects the value of the option to invest in CCS.

$$F_1(E) = A_1 \cdot E^{\beta_1}. \tag{8}$$

The optimal CO_2 price threshold to invest in CCS, E^*_{ccs} and the constant A_1 are obtained analytically by applying value-matching and smooth-pasting between (5) and (8). The solution procedure is presented in Appendix A.1. Then E^*_{ccs} and A_1 are equal to:

$$E^*_{ccs,1} = \frac{\beta_1}{\beta_1 - 1}\left(\frac{\rho-\alpha}{\rho}\cdot(C_c + C_{ts}) + \frac{\rho-\alpha}{Q_{co_2}}\cdot I_c\right), \tag{9}$$

$$A_1 = \frac{Q_{co_2}}{\rho-\alpha}\cdot\frac{1}{\beta_1}\left(\frac{\beta_1}{\beta_1 - 1}\left(\frac{\rho-\alpha}{\rho}\cdot(C_c + C_{ts}) + \frac{\rho-\alpha}{Q_{co_2}}\cdot I_c\right)\right)^{\beta_1}. \tag{10}$$

In sum, as long as the CO_2 price is lower than E^*_{ccs}, the value of waiting (8) is greater than the project value (5). Once the CO_2 price crosses the threshold E^*_{ccs}, the firm invests: the option value and the project value coincide.

2.2 Model 2: Simultaneous CCUS

Next, we assume that the firm is operating in the dark purple region in Figure 4, where it is optimal to invest in CCUS. In Model 2, CCU starts to play a role, and hence, the unknown arrival of CCU now needs to be considered. The investment decision is split into two stages: one before and one after CCU arrival. In Stage 1, before CCU arrives, the firm might decide to not wait any longer and invest in CCS already. We will show that there exists a CO_2 price $E^*_{ccs,1}$ that triggers optimal investment in CCS in Stage 1, taking into account the expected arrival of CCU in the future. In Stage 2, once CCU has arrived, a new investment decision problem emerges. If CCU arrives and the firm already invested in CCS in Stage 1, the firm adopts CCU immediately upon its arrival. If, however, CCU arrives and the firm did not invest yet in Stage 1, we will show that there exists a CO_2 price $E^*_{ccus,2}$ that triggers optimal investment in CCUS in Stage 2. The outlined sequence of actions in Model 2 corresponds to adoption strategies (S.2) and (S.4) in Figure 2: investing in CCS in Stage 1 and in CCU when it arrives (S.2) and investing in CCUS in Stage 2 (S.4).

Figure 5 summarizes this two-staged problem from Model 2, with a different type of investment decision in each stage. Depending on the stage and depending on the actions that were previously taken, the firm will face a different type of investment decision, with different CO_2 price thresholds to be found. Four different value functions are identified:

1. $F_1(E)$: Initially, the firm is in Stage 1, where the CCU technology has not yet entered the market. Hence, the firm holds an option to invest in CCS and an option to adopt CCU, once it leaves the R&D phase and enters the market as well.
2. $\phi_1(E)$: If the CO_2 price exceeds the threshold $E^*_{ccs,1}$ before the CCU technology arrives, the firm will invest in CCS first. The firm then holds the value function $\phi_1(E)$, which represents the value of operating CCS and the option to adopt CCU, once CCU enters the market.
3. $\phi_2(E)$: The firm has invested in CCS and now the CCU technology becomes available, i.e. the firm transitions from Stage 1 to Stage 2. The firm now holds the value function $\phi_2(E)$, which is the value of operating CCUS.

4. $F_2(E)$: If, on the other hand, the CCU technology enters the market before the CCS technology is adopted, the firm transitions to Stage 2 first. The firm now holds the value function $F_2(E)$, which includes an option to invest in CCUS simultaneously.

These value functions and the optimal investment thresholds are now analyzed through backward induction, starting in Stage 2. We will now apply the dynamic programming technique, as described in Dixit and Pindyck (1994), to find the option value and the investment thresholds $E^*_{ccs,1}$ and $E^*_{ccus,2}$.

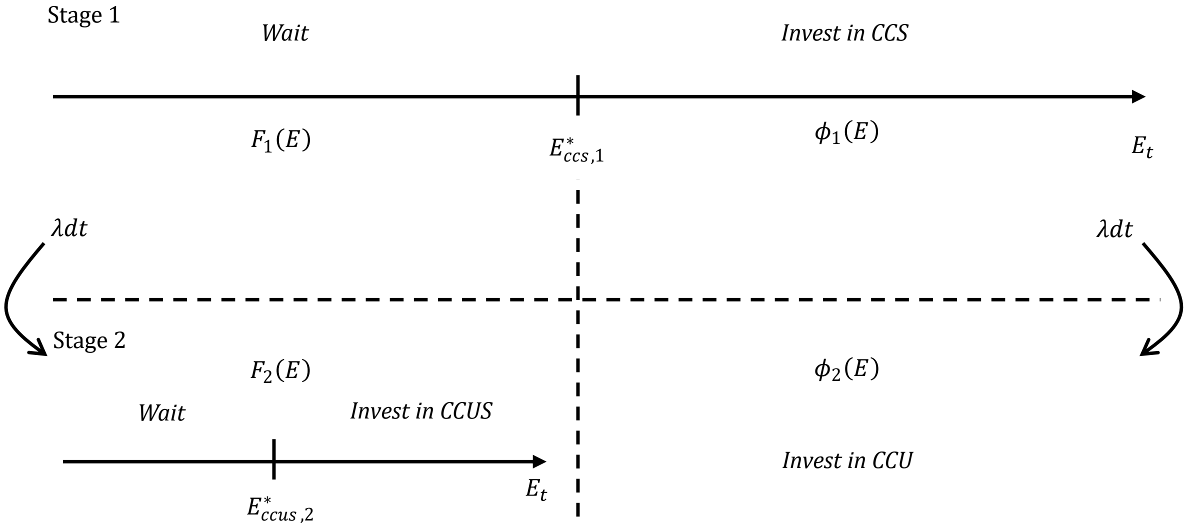


Figure 5: The two-staged decision problem for the firm, in Model 2.

2.2.1 Stage 2

In Stage 2, the CCU technology is mature and ready to install, leaving the firm with only one source of uncertainty: the CO_2 price uncertainty.

We first assume that the firm invests in CCS in Stage 1 and is now operating CCS (upper right box in Figure 5). In this case, all CO_2 emissions are captured and stored. Hence, no more emission allowances need to be paid and the CO_2 price uncertainty is completely resolved as well. As a result, when CCU arrives (lower right box in Figure 5), the firm will immediately adopt the CCU technology. The firm's value then equals the value of operating CCUS, V_{ccus}:

$$\phi_2(E) = \frac{Q_{co_2}}{\rho - \alpha} \cdot E - \frac{Q_{co_2}}{\rho} \cdot C_c - \frac{(1-q)Q_{co_2}}{\rho} * C_{ts} + \frac{q \cdot Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_u) - I_c - I_u. \tag{11}$$

If, on the other hand, the firm waited in Stage 1, a new optimal investment problem starts in Stage 2. In this case (lower left box in Figure 5), it is optimal to invest in CCUS simultaneously. The threshold $E^*_{ccus,2}$ characterizes the optimal time to invest.

When $E > E^*_{ccus,2}$, the firm invests in CCUS and gains the project value V_{ccus} (4).

As long as $E \leq E^*_{ccus,2}$, the firm waits and holds on to the option to invest in CCUS. Using similar steps as described in Dixit and Pindyck (1994), the option value can be derived. First, the Bellman equation for this option value in Stage 2 is

$$\rho \cdot F_2(E) = \lim_{dt \to 0} \frac{1}{dt} \cdot \mathbb{E}[dF_2]. \tag{12}$$

The Bellman equation in (12) is now expanded using Ito's Lemma, which results in the ODE

$$\frac{1}{2}\sigma^2 E_t^2 F_2^{"}(E) + \alpha E F_2'(E) - \rho F_2(E) = 0. \tag{13}$$

This ODE is similar to the ODE in Model 1 (7) and hence, the same steps are followed to find its solution. The value of the option to invest in CCUS can be found in (A.6) and the optimal investment threshold $E^*_{ccus,2}$ and the constant $A_{1,sim}$ are given by:

$$E^*_{ccus,2} = \frac{\beta_1}{\beta_1 - 1}\left(\frac{\rho - \alpha}{\rho} \cdot (C_c + (1-q) \cdot C_{ts} - q \cdot (P \cdot X - C_u)) - \frac{\rho - \alpha}{Q_{co_2}} \cdot (I_c + I_u)\right), \tag{14}$$

$$A_{1,sim} =$$
$$\frac{Q_{co_2}}{\rho - \alpha}\frac{1}{\beta_1} \cdot \left[\frac{\beta_1}{\beta - 1} \cdot (\frac{\rho - \alpha}{\rho} \cdot (C_c + (1-q) \cdot C_{ts} - q * (P_p \cdot X - C_u)) - \frac{\rho - \alpha}{Q_{co_2}} \cdot (I_c + I_u)\right]^{1-\beta_1}. \tag{15}$$

The proof for these equations can be found in Appendix A.2.

2.2.2 Stage 1

In Stage 1, the timing of the CCU arrival is still unknown and the firm needs to consider both the market and technological uncertainty in its investment decision. Similar to Model 1, the firm wants to find the threshold $E^*_{ccs,1}$, which defines the optimal investment timing in CCS. Unlike Model 1, the firm now also needs to take the value of the option to invest in CCU(S) in Stage 2 into account.

When $E > E^*_{ccs,1}$ before CCU arrives (upper right in Figure 5), the firm invests in CCS and earns the project value $V_{ccs}(E)$ (2). As described before, the firm will adopt CCU when it arrives in this case. As a result, $\phi_1(E)$ needs to reflect both the value of operating CCS now and the value of operating CCU once it arrives:

$$\phi_1(E) = \frac{Q_{co_2}}{\rho - \alpha} \cdot E - \frac{Q_{co_2}}{\rho} \cdot (C_c + C_{ts}) - I_c + \frac{\lambda}{\lambda + \rho} \cdot (\frac{q \cdot Q_{co_2}}{\rho} \cdot (P_p \cdot X + C_{ts} - C_u) - I_u). \tag{16}$$

The expression for $\phi_1(E)$ contains the expected profit from operating both CCS and CCU. However, the value from operating CCU is adjusted by the term $\frac{\lambda}{\lambda+\rho}$, since CCU has not arrived yet.

As long as $E < E^*_{ccs,1}$ (upper left box in Figure 5), it is still optimal to wait with the investment. The firm now holds an option to invest in CCS (before CCU arrives) and to invest in CCU simultaneously (once CCU arrives). Let $F_1(E)$ denote the value of the option that the firm is holding in Stage 1, along with all future options. To describe $F_1(E)$, we follow similar steps as in Dixit and Pindyck (1994) (p. 202-205) and Sendstad and Chronopoulos (2020). When $E < E^*_{ccs,1}$, no profits are earned yet. With a probability λdt, CCU arrives in the next short time interval dt. The firm then moves to Stage 2 and holds the option worth $F_2(E)$ (A.6). With a probability $1 - \lambda dt$, CCU does not arrive yet and the firm continues to hold $F_1(E)$. This gives the following dynamics for the value function $F_1(E)$ over a small interval of time dt:

$$F_1(E) = (1 - \lambda dt)\mathbb{E}[F_1(E + dE)]e^{-\rho dt} + \lambda dt \mathbb{E}[F_2(E + dE)]e^{-\rho dt}, \tag{17}$$

Expanding the right-hand side of this equation using Ito's Lemma (A.10), results in the ODE

$$\frac{1}{2}\sigma^2 E^2 F_1^{''}(E) + \alpha E F_1^{\prime}(E) - \rho \cdot F_1(E) + \lambda \cdot (F_2(E) - F_1(E)) = 0. \tag{18}$$

The main difference with the previous ODE in (7) and (13) is the additional term $\lambda \cdot (F_2(E) - F_1(E))$, which is added to reflect that the value of the option can switch from $F_1(E)$ to $F_2(E)$ if CCU arrives while the firm waits. Because of this additional term $\lambda F_2(E)$, the solution for $F_1(E)$ will consist of a homogeneous and a particular solution. Note that $F_2(E)$ is defined differently over two CO_2 price intervals, i.e. $E \leq E_{ccus,2^*}$ and $E > E^*_{ccus,2}$. Hence, we must solve (18) separately for these two price intervals as well. The solution for $F_1(E)$ is indicated in (19). The first part of $F_1(E)$, $C_{1,sim} \cdot E^{\delta_1}$, reflects the option to invest in CCS alone, prior to CCU arrival, while the second part within brackets reflects the option to invest in CCUS, after CCU arrival.

$$\begin{aligned} F_1(E) = {} & C_{1,sim} \cdot E^{\delta_1} + \\ & \begin{cases} A_{1,sim} \cdot E^{\beta_1} + B_1 \cdot E^{\delta_1} \quad \text{if} \quad E \leq E^*_{ccus,2}, \\ \frac{\lambda}{\lambda+\rho-\alpha} \frac{Q_{co_2}}{\rho-\alpha} \cdot E + \frac{\lambda}{\lambda+\rho} [-\frac{Q_{co_2}}{\rho} \cdot C_c - \frac{(1-q)Q_{co_2}}{\rho} \cdot C_{ts} + \frac{q \cdot Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_u) - I_c - I_u] \\ +B_4 \cdot E^{\delta_2} \quad \text{if} \quad E > E^*_{ccus,2}. \end{cases} \end{aligned} \tag{19}$$

The first term on the top part of (19) represents the option to invest in CCUS, adjusted via the second (negative) term because CCU has yet to arrive. The first terms on the bottom part represent the value of operating CCUS, adjusted by λ. The final term indicates the likelihood that the CO_2 price may drop back to a level below $E^*_{ccus,2}$, before the CCU technology arrives. The constants $A_{1,sim}$ and the threshold $E^*_{ccus,2}$ were given in (15) and (14). The constants B_1 and B_4 are determined analytically through value-matching (A.11) and smooth pasting conditions (A.12) at the threshold $E^*_{ccus,2}$. The terms δ_1 and δ_2 are the positive and negative roots of the quadratic equation $\frac{1}{2}\sigma^2\delta^2 + (\sigma - \frac{1}{2}\sigma^2)\delta - (\rho + \lambda) = 0$. The constant C_1 and the investment threshold $E^*_{ccs,1}$ are found by applying value-matching and smooth-pasting at the threshold $E^*_{ccs,1}$, where $F_1(E)$ and $\phi_1(E)$ should match.

2.3 Model 3: Sequential CCU - CCS

Next, consider the region where it is optimal to invest in CCU and CCS sequentially (light purple region in Figure 4). The real options model for this scenario is very similar to Model 2, with one major difference: instead of finding one investment threshold $E^*_{ccus,2}$, the firm now needs to identify two thresholds $E^*_{ccu,2}$ and $E^*_{ccs,2}$. Model 3 describes the optimal timing to invest in CCS and CCU for adoption strategies (S.2) and (S.5) in Figure 2.

Figure 6 summarizes the firm's decision problem for Model 3. The sole difference with Model 2 is in $F_2(E)$, which now describes the value of the option to invest in CCU and CCS sequentially. Analogous to Model 2, the optimal investment thresholds $E^*_{ccs,1}$, $E^*_{ccu,2}$ and $E^*_{ccs,2}$ are determined through backward induction. In this section, only the differences with Model 2 will be highlighted.

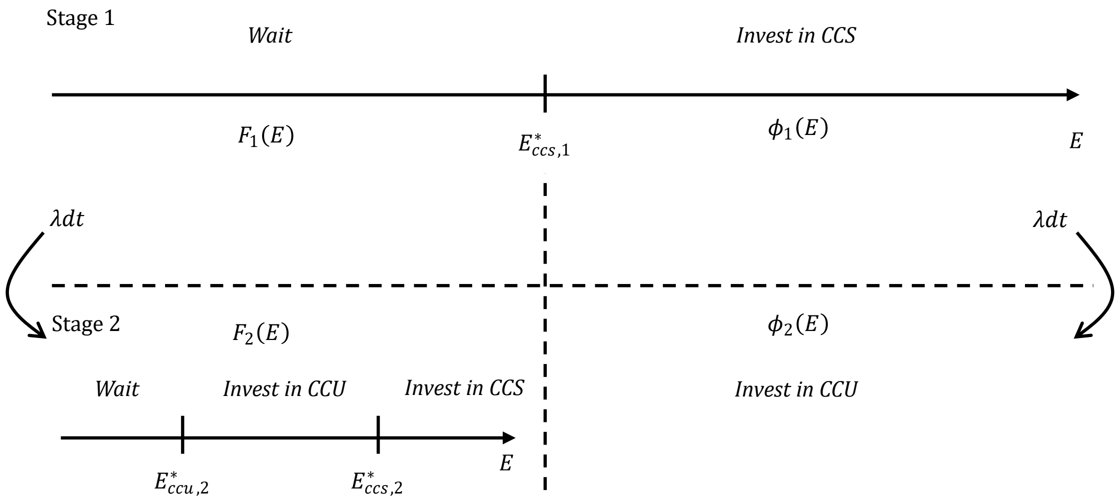


Figure 6: The two-staged decision problem for the firm, in Model 3.

2.3.1 Stage 2

If the firm adopted CCS in Stage 1 (lower right corner in Figure 6), it will immediately install CCU in Stage 2, as discussed before. The firm obtains $\phi_2(E)$, equal to the value of operating CCUS (4).

If, on the other hand, the firm waited in Stage 1 until CCU entered the market (lower left corner in Figure 6), the firm's optimal strategy is now to adopt CCU and CCS in a sequential manner. Therefore, the firm now needs to find two investment thresholds (instead of one) to determine the optimal timing of the investments in respectively CCU and CCS: $E^*_{ccu,2}$ and $E^*_{ccs,2}$.

As long as $E < E^*_{ccu,2}$, the firm continues to wait and holds the option to invest in CCU and CCS sequentially. The Bellman equation (12) and the resulting ODE (13) are identical to the solutions in Model 2, when $E < E^*_{ccus,2}$. The solution for the ODE when $E < E^*_{ccu,2}$ is $F_2(E) = A_{1,seq} \cdot E^{\beta_1}$.

When $E^*_{ccu,2} \leq E \leq E^*_{ccs,2}$, the firm invests in CCU but continues to wait with the investment in CCS. This results in a new Bellman equation that includes the profits from operating CCU:

$$\rho F_2(E) = \pi_{ccu} + \lim_{dt \to 0} \frac{1}{dt} \mathbb{E}[dF_2], \tag{20}$$

In this equation, π_{ccu} reflects the net earnings the firm receives from operating CCU. This equals the present value V of the CCU technology, presented in (3), but excluding the investment costs I_u and I_c, because π_{ccu} reflects the net returns from operating CCU after investment. Expanding this new Bellman equation (20) using Ito's lemma, we obtain the ODE

$$\frac{1}{2}\sigma^2 E^2 F_2^{''} + \alpha E F_2^{'} - \rho F_2 + \pi_{ccu} = 0. \tag{21}$$

The general solution of this ODE will now consist of a homogeneous and a particular solution, due to the additional term π_{ccu}. Hence, the solution for the ODE in (21) is

$$F_2(E) = D_1 \cdot E^{\beta_1} + \frac{q \cdot Q_{co_2}}{\rho - \alpha} \cdot E + \frac{q \cdot Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_c - C_u) - I_c - I_u, \tag{22}$$

where the first part reflects the option to invest in CCS and the second part reflects the expected present value of the profits from operating CCU.

Finally, when $E > E^*_{ccs,2}$, the firm also adopts CCS and starts operating CCUS. The value function $F_2(E)$ now equals the CCUS profits in (4).

The solution for $F_2(E)$ over the three CO_2 price intervals is shown in (23)

$$F_2(E) = \begin{cases} A_{1,seq} \cdot E^{\beta_1} \quad \text{if} \quad E < E^*_{ccu,2}, \\ D_1 \cdot E^{\beta_1} + \frac{q \cdot Q_{co_2}}{\rho - \alpha} \cdot E + \frac{q \cdot Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_c - C_u) - I_c - I_u \quad \text{if} \quad E^*_{ccu,2} \leq E \leq E^*_{ccs,2}, \\ \frac{Q_{co_2}}{\rho - \alpha} \cdot E - \frac{Q_{co_2}}{\rho} \cdot C_c - \frac{(1-q) \cdot Q_{co_2}}{\rho} \cdot C_{ts} + \frac{q \cdot Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_u) - I_c - I_u \quad \text{if} \quad E > E^*_{ccs,2}. \end{cases} \tag{23}$$

The solutions for $E^*_{ccu,2}$ and $E^*_{ccs,2}$ are found via value-matching ((A.13) and (A.15)) and smooth pasting ((A.14) and (A.16)) conditions between the three branches of (23). The solutions for the constants $A_{1,seq}$ and D_1 can be found in Appendix A.3.

$$E^*_{ccu,2} = \frac{\beta_1}{\beta_1 - 1} \cdot (\frac{\rho - \alpha}{\rho} \cdot (C_c + C_u - P_p \cdot X) + \frac{\rho - \alpha}{q \cdot Q_{co_2}} \cdot (I_c + I_u)), \tag{24}$$

$$E^*_{ccs,2} = \frac{\beta_1}{\beta_1 - 1} \cdot \frac{\rho - \alpha}{\rho} \cdot (C_c + C_{ts}). \tag{25}$$

The CO_2 price investment threshold for CCU depends on the capture costs, utilization costs, the product price, the conversion rate and the investment costs for the capture facility and the utilization plant (24). The investment threshold for CCS, when the firm is already operating CCU, is only affected by the capture costs and the transport and storage fee (25). Note that the investment for the capture plant I_c does not affect the threshold for CCS, as this investment cost was already incurred to adopt CCU. As can be seen from (25), the capture cost C_c per tonne of captured CO_2 is included in the CO_2 price threshold to invest in CCS. When the firm adopts CCU first, only part of its CO_2 emissions are captured and utilized, due to its limitations in scale. As a result, only when the firm also adopts CCS, all of the firm's CO_2 emissions are captured. Hence, the costs to capture these additional amounts of CO_2 need to be accounted for and are reflected in the threshold to invest in CCS, with the presence of C_c, the capture cost per tonne of CO_2 captured.

2.3.2 Stage 1

In stage 1, CCU is still in the R&D phase and it is yet unknown when CCU will enter the market.

When $E > E^*_{ccs,1}$ before CCU arrives (upper right corner in Figure 6), the firm invests in CCS and obtains the profits from operating CCS (2). Because the CO_2 price uncertainty is now resolved, the firm will also adopt CCU immediately when it arrives. Hence, $\phi_1(E)$ equals the sum of the profits from CCS and the expected profits from CCU in the future, as shown in Model 2 (16).

As long as $E \leq E^*_{ccs,1}$ (upper left corner in Figure 6), the firm waits and holds the option to invest in CCU and CCS. Following the steps from Dixit and Pindyck (1994), results in the same ODE as in Model 2 (18). However, $F_2(E)$ is now defined over three different intervals, i.e. $E < E^*_{ccu,2}$, $E^*_{ccu,2} \leq E \leq E^*_{ccs,2}$ and

$E > E^*_{ccs,2}$. The solution for $F_1(E)$ over all CO$_2$ price intervals is presented in (26). The first part, $C_{1,seq} * E^{\delta_1}$, again reflects the option to invest in CCS before CCU arrives, while the second part reflects the option to invest in CCU and CCS sequentially after CCU arrived.

$$
\begin{aligned}
&F_1(E) = C_{1,seq} \cdot E^{\delta_1} + \\
&\begin{cases}
A_{1,seq} \cdot E^{\beta_1} + B_{1,seq} \cdot E^{\delta_1} & \text{if} \quad E < E^*_{ccu,2}, \\
\frac{\lambda}{\rho+\lambda-\alpha} \cdot \frac{q * Q_{co_2}}{\rho-\alpha} \cdot E + \frac{\lambda}{\lambda+\rho} \cdot \left[\frac{q * Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_u - C_c) - I_c - I_u\right] + & \\
D_1 \cdot E^{\beta_1} + B_{2,seq} \cdot E^{\delta_1} + B_{3,seq} \cdot E^{\delta_2} & \text{if} \quad E^*_{ccu,2} \leq E \leq E^*_{ccs,2}, \\
\frac{\lambda}{\rho+\lambda-\alpha} \cdot \frac{q * Q_{co_2}}{\rho-\alpha} \cdot E + \frac{\lambda}{\lambda+\rho} \cdot \big[- \frac{Q_{co_2}}{\rho} \cdot C_c - (1-q) Q_{co_2} \cdot C_{ts} + & \\
\frac{q \cdot Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_u) - I_c - I_u \big] + B_{4,seq} \cdot E^{\delta_2} & \text{if} \quad E > E^*_{ccs,2}.
\end{cases}
\end{aligned}
\tag{26}
$$

The first term in the top part of (26) represent the option to invest in CCU, adjusted for the unknown arrival timing of CCU by the second term. The first two terms in the middle part of (26) represent the expected present value of the CCU profits. The third term reflects the option to invest in CCS, adjusted via the fourth term because CCU hasn't arrived yet. The fifth term accounts for the possibility that the CO$_2$ price drops below $E^*_{ccu,2}$ before CCU arrives. The first two terms in the bottom part of (26) are the expected profits from operating CCUS, adjusted for the possibility that the CO$_2$ price drops below $E^*_{ccs,2}$ by the third term. The constants $A_{1,seq}$ and D_1 and the investment thresholds E^*_{ccu} and $E^*_{ccs,2}$ are the same as in $F_2(E)$ (A.7). The constants $B_{1,seq}$, $B_{2,seq}$, $B_{3,seq}$ and $B_{4,seq}$ are found by applying the value-matching and smooth-pasting conditions between the three branches of $F_1(E)$ (A.20)-(A.23). The constant $C_{1,seq}$ and the threshold $E^*_{ccs,1}$ are obtained by applying value matching and smooth pasting to $F_1(E)$ and $\phi_1(E)$ at $E^*_{ccs,1}$.

2.4 Model 4: Immediate CCU - later CCS

Finally, we analyze the optimal investment timing in the blue area in Figure 4, where the firm immediately invests in CCU, once it arrives. In Stage 1, the firm invests in CCS if $E > E^*_{ccs,1}$. In Stage 2, the firm adopts CCU immediately upon its arrival. When the CO$_2$ price continues to rise, the incentive to avoid all CO$_2$ becomes larger, and the firm will also adopt CCS in Stage 2. This possible sequence of investment decisions matches adoption strategies (S.2) and (S.6) in Figure 2.

Figure 7 shows how the investment decision problem in Model 4 evolves over both stages. The value functions $\phi_1(E)$ and $\phi_2(E)$ are the same as in Models 2 and 3, while the value functions $F_1(E)$ and $F_2(E)$ are defined slightly different compared to the previous models:

1. $F_1(E)$: the firm holds an option to invest in CCS and an option to invest in CCU, once it arrives, followed by CCS investment, when the CO$_2$ price is high enough.
2. $F_2(E)$: if CCU matures before the firm invested in CCS, the firm will immediately invest in CCU and hold an option to invest in CCS later, when CO$_2$ prices continue to rise.

The optimal investment thresholds $E^*_{ccs,1}$ and $E^*_{ccs,2}$ are again determined using backward induction.

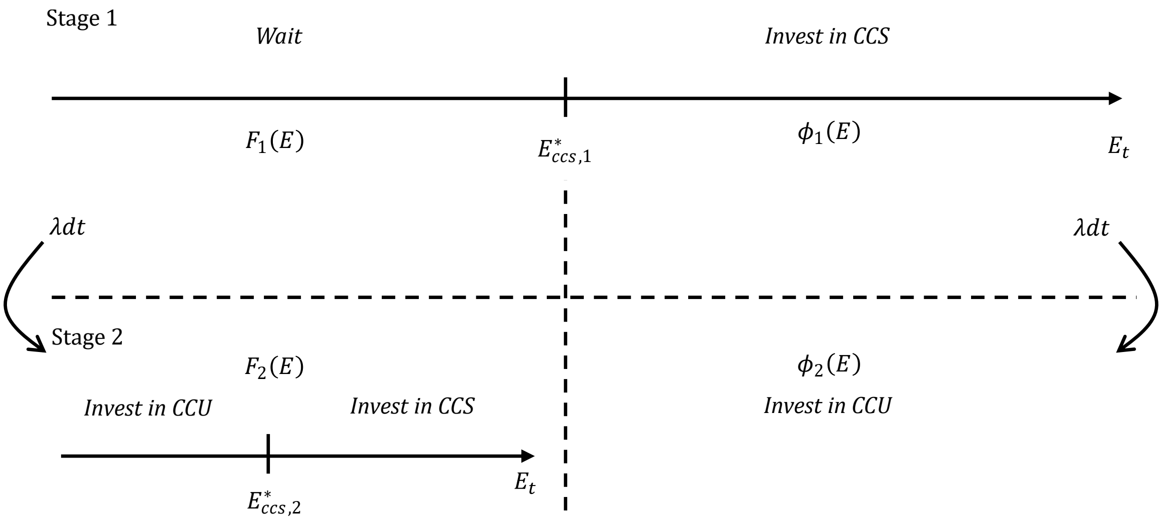


Figure 7: The two-staged decision problem for the firm, in Model 4.

2.4.1 Stage 2

If the firm already invests in CCS in Stage 1(lower right corner in Figure 7), the firm's value function $\phi_2(E)$ again equals the expected present value of the CCUS profits (4). Even if the firm did not yet invest in CCS, the firm is now triggered to invest in CCU when it arrives, independent of the CO$_2$ price. Hence, there is only one investment threshold, $E^*_{ccs,2}$.

The investment threshold $E^*_{ccs,2}$ will define the optimal timing for the investment in CCS. The Bellman equation is

$$\rho \cdot F_2(E) = \pi_{ccu} + \lim_{dt \to 0} \frac{1}{dt} \cdot \mathbb{E}[dF_2]. \tag{27}$$

which is the same Bellman equation as in Model 3, when $E^*_{ccu,2} \leq E \leq E^*_{ccs,2}$ (20). As a result, the ODE (21) and the solution for this ODE (22) are also the same as in Model 3.

We get the following expression for $F_2(E)$ in Model 4

$$F_2(E) = \begin{cases} A_{1,imm} \cdot E^{\beta_1} + \frac{q \cdot Q_{co_2}}{\rho - \alpha} E + \frac{q \cdot Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_c - C_u) - I_c - I_u & \text{if} \quad E \leq E^*_{ccs,2}, \\ \frac{Q_{co_2}}{\rho - \alpha} \cdot E - \frac{Q_{co_2}}{\rho} \cdot C_c - \frac{(1-q) \cdot Q_{co_2}}{\rho} C_{ts} + \frac{q \cdot Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_u) - I_c - I_u & \text{if} \quad E > E^*_{ccs,2}. \end{cases} \tag{28}$$

The threshold $E^*_{ccs,2}$ and the constant $A_{1,imm}$ are obtained through value-matching and smooth-pasting at the threshold. Since these conditions are the same as in Model 3 ((A.15) and (A.16)), the investment threshold $E^*_{ccs,2}$ and the constant $A_{1,imm}$ are also identical to the threshold $E^*_{ccs,2}$ (25) and the constant $A_{1,seq}$ (A.17) in Model 3.

2.4.2 Stage 1

In Stage 1, the arrival timing of CCU is still unknown and the firm needs to determine the optimal investment timing for CCS.

When $E > E^*_{ccs,1}$, the firm invests in CCS and obtains $\phi_1(E)$ (16), representing the expected profits from operating CCS and CCU.

As long as $E \leq E^*_{ccs,1}$, the firm waits and holds the option to invest in CCS (before CCU arrives) and the option to invest in CCU when it arrives, and CCS at high enough CO_2 prices. The Bellman equation is

$$\rho \cdot F_1(E) = \frac{1}{dt}\mathbb{E}[dF_1]. \tag{29}$$

Expanding the Bellman equation by applying Ito's Lemma, results in the same ODE as in Models 3 and 2 (18). Since $F_2(E)$ is defined over two different CO_2 price intervals, $F_1(E)$ must be solved for these intervals separately, i.e. $E \leq E^*_{ccs,2}$ and $E > E^*_{ccs,2}$. The solution for $F_1(E)$ over both CO_2 price intervals is presented in (30).

$$\begin{aligned} F_1(E) = {} & C_{1,imm} \cdot E^{\delta_1} + \\ & \begin{cases} A_{1,imm} \cdot E^{\beta_1} + \frac{\lambda}{\lambda+\rho-\alpha}\frac{q \cdot Q_{co_2}}{\rho-\alpha} \cdot E + \frac{\lambda}{\lambda+\rho} + \frac{q \cdot Q_{co_2}}{\rho} \cdot [(P_p \cdot X - C_c - C_u) - I_c - I_u] + \\ B_{1,imm} \cdot E^{\delta_1} \quad \text{if} \quad E \leq E^*_{ccs,2}, \\ \frac{\lambda}{\lambda+\rho-\alpha}\frac{Q_{co_2}}{\rho-\alpha} \cdot E + \frac{\lambda}{\lambda+\rho} \cdot [-\frac{Q_{co_2}}{\rho} \cdot C_c - \frac{(1-q) \cdot Q_{co_2}}{\rho} \cdot C_{ts} + \frac{q \cdot Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_u) - I_c - I_u] \\ +B_{4,imm} \cdot E^{\delta_2} \quad \text{if} \quad E > E^*_{ccs,2}. \end{cases} \end{aligned} \tag{30}$$

The first part, $C_{1,imm} \cdot E^{\delta_1}$, again reflects the option to invest in CCS, before CCU arrives. The second part, between brackets, represents the option to invest in CCU and CCS, once CCU has arrived. Analogous to the previous models, the term $B_1 \cdot E^{\delta_1}$ is added to adjust for the unknown arrival of CCU and the term $B_4 \cdot E^{\delta_2}$ accounts for the possibility that the CO_2 price again drops below $E^*_{ccu,2}$ before CCU arrives. The constants $B_{1,imm}$ and $B_{4,imm}$ are found via the value-matching and smooth pasting conditions between the two branches of $F_1(E)$ (A.24)-(A.25). The constant $C_{1,imm}$ and the threshold $E^*_{ccs,1}$ are obtained by applying value matching and smooth pasting to $F_1(E)$ and $\phi_1(E)$ at $E^*_{ccs,1}$.

3 A numerical example: the cement industry

In this section, the real options models are applied to three CCUS scenarios in the cement industry, based on the economic feasibility study by Monteiro and Roussanaly (2022). The CO_2 source is a cement plant that produces 1.36 Mt cement per year and emits 771,000 tonnes of CO_2 annually. The investigated CO_2 utilization pathways in the CCUS chains are the conversion of CO_2 to ethanol as a fuel, the direct use of CO_2 as food-grade CO_2, and the conversion of CO_2 to polyol as polymer feedstock. The cement plant emits more CO_2 than can be used in any of these CCU pathways, either due to market size or to availability of other raw materials. Therefore, if the aim is to abate all CO_2 emissions from the cement plant, CCS and CCU should be used as complementary solutions in a CCUS chain. Hence, the CCUS scenarios in Monteiro and Roussanaly (2022) fit the framework of the real options model that was developed in this study. The parameters for each CCUS scenario are summarized in Table 2. The three CCUS scenarios differ in the investments for the utilization plant I_u, the utilization costs C_u, the price of the product P_p, the conversion factor from CO_2 to final product X and the arrival rate λ. The ethanol production route has the lowest maturity level, which results in a slower arrival rate λ than the food-grade CO_2 or polyol production route. As can be seen from Table 2, the fractions of CO_2 that can be utilized, q, is rather low in all three scenarios. The amount of CO_2 that can be utilized in a CCU route can be limited due to the market size of the product or due to technical limitations. For the ethanol CCUS chain, it is the need for large amounts of renewable hydrogen that limits its CO_2 utilization capacity. For the CCUS value chains with food-grade CO_2 and polyol as products, the amount of CO_2 that can be utilized is limited by the market for the product.

One of the underlying assumptions of the real options model is that the same actor invests in the CO_2 capture and the CO_2 utilization technology. While it may seem irrelevant for a cement plant to invest in the utilization of CO_2 for the production of e.g. ethanol, examples can be found of firms that invest in CCU plants to be built on their site, even if the CCU-product is not within their core industry. For example, ArcelorMittal, a steel company, has invested in the development of a CCU installation that will capture CO_2 emissions from a steel plant and convert the CO_2 into bioethanol, to be sold to the transportation sector (ArcelorMittal, 2023).

Figure 8 shows the present values from the investment in CCS, CCU or CCUS for each scenario from Table 2. In the ethanol CCUS scenario, the CCS technology always yields the highest value, compared to CCUS and CCU. When the CO_2 is used as food-grade CO_2, the CCU solution reaches break-even first, closely followed and overpowered by the combined CCUS technology. In the polyol CCUS chain, CCU already yields a positive present value at a zero CO_2 price.

Parameter	**Ethanol**	**Food-grade CO_2**	**Polyol**	**Unit**	**Reference**
TRL	5	9	9		
Q_{co_2}	771,000	771,000	771,000	t CO_2/year	
q	3.1	6.5	7.5	%	
I_c	15,000,000	15,000,000	15,000,000	€	(Gardarsdóttir et al., 2018)
I_u	22,600,000	16,000,000	21,000,000	€	
C_c	69	69	69	€/ton CO_2	
C_{ts}	20	20	20	€/ton CO_2	(Jang et al., 2016)
C_u	656	100	603*	€/ton CO_2	*(Fernández-Dacosta et al., 2017)
P_p	633	150	1400	€/ton product	
X	0.525	1	5		
ρ	8	8	8	%	(Gardarsdóttir et al., 2019)
α	0.05	0.05	0.05		(Compernolle et al., 2017)
σ	0.2	0.2	0.2		(Compernolle et al., 2017)
λ	0.2	0.5	0.5		

Table 2: Description of three CCUS scenarios for the cement industry: ethanol production (fuel), food-grade CO_2 production (direct use of CO_2) and polyol production (chemical). The numbers for the three scenarios are based on Monteiro and Roussanaly (2022), unless indicated otherwise.

Figure 8 reflects how the differences in costs and revenues, as listed in Table 2, cause variations in which of the technologies presents the most profitable solution. This will also affect the optimal adoption strategy of the firm for each scenario.

Figure 9 presents the positioning of each CCUS scenario in its optimal region (as previously shown in Figure 4). The ethanol CCUS scenario is located in the red region, where it is the most profitable to invest only in CCS (Model 1). For the food-grade CO_2 CCUS chain, the optimal strategy is to adopt CCU and CCS sequentially (Model 3). Finally, the polyol CCUS chain is in the blue region, where CCU is so profitable that the firm will immediately adopt CCU upon arrival. When the CO_2 price reaches a certain threshold, the firm will also abate the remaining CO_2 emissions with CCS (Model 4). Following the Models 1, 3 and 4, we can now calculate the actual CO_2 price levels at which the firm should invest in each technology.

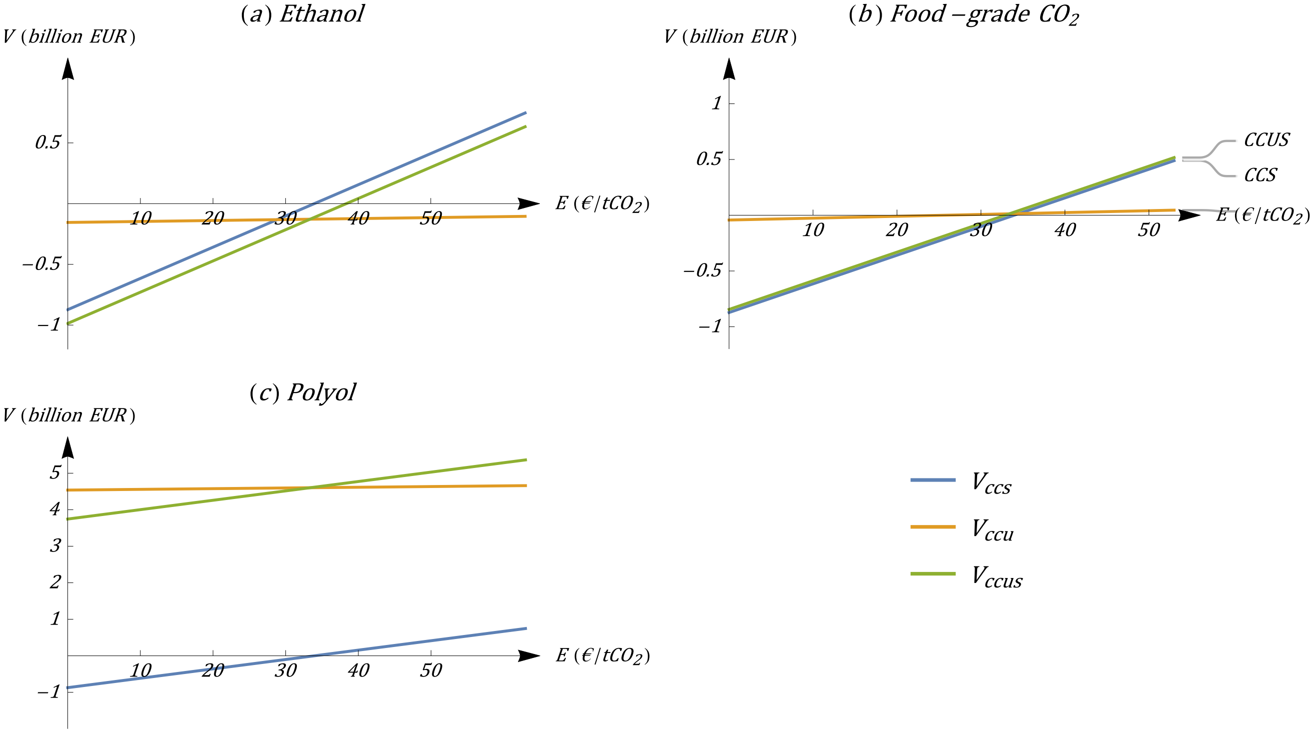


Figure 8: The present values of the CCS (blue), CCU (orange) and CCUS (green) solutions in each CCUS scenario based on Monteiro and Roussanaly (2022), (a) the conversion of CO_2 into ethanol as CCU route, (b) the direct use of CO_2 as food-grade CO_2, and (c) the conversion of CO_2 into polyol.

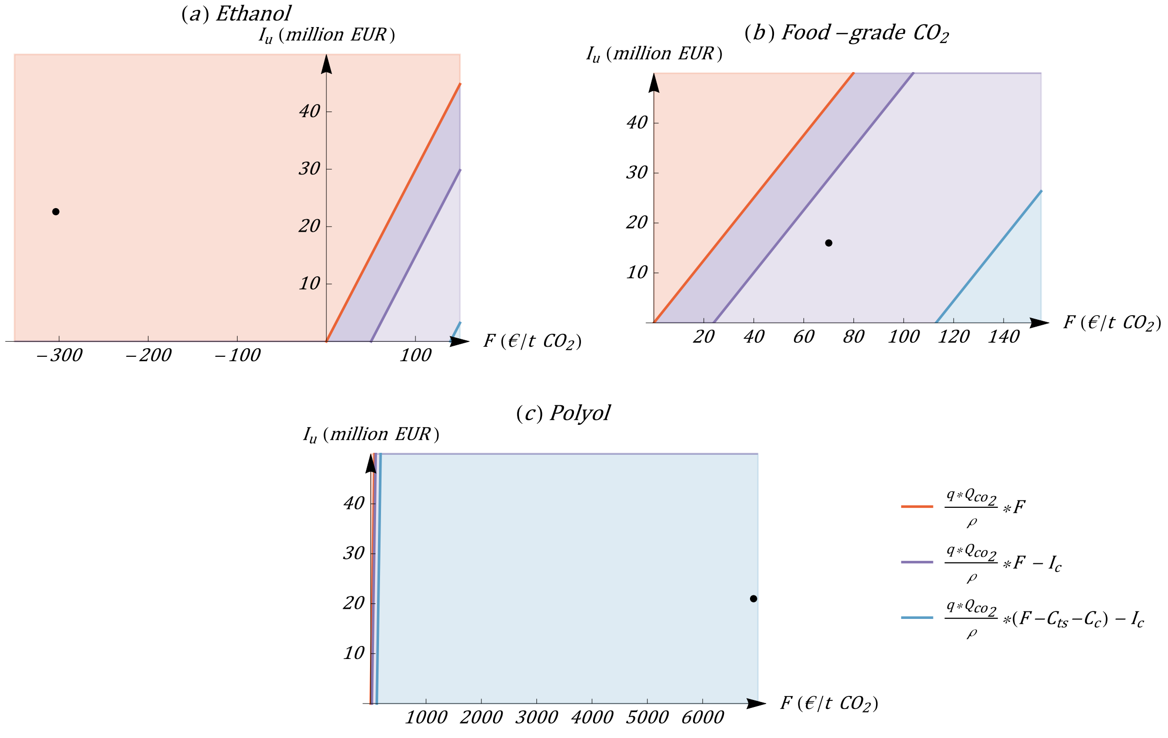


Figure 9: The optimal region for each CCUS scenario (a) ethanol (q = 0.031), (b) food-grade CO_2 (q = 0.065), and (c) polyol (q = 0.075) represented by the black dot.

3.1 Model 1: Ethanol production

Model 1, as developed in Section 2.1, is applied to the ethanol CCUS chain to identify the optimal investment timing. Because the investment in CCS always results in higher value than the investment in CCU or CCUS (Figure 8), only one CO_2 price threshold needs to be found: $E^*_{ccs,1}$, the CO_2 price threshold to invest in CCS. Figure 10 shows the results of Model 1 for the ethanol CCUS chain. The firm should invest in CCS once the CO_2 price exceeds 121.9 €/t CO_2.

3.2 Model 3: Food-grade CO_2 production

Because of the higher fraction of CO_2, q, that can be used for food-grade CO_2, the lower investment costs, I_u, and higher conversion rate, X, it can be valuable to invest in CCU in the food-grade CO_2 CCUS chain. Figure 8 shows how the sequential CCU-CCS adoption strategy is optimal, once the CCU technology is mature. Therefore, Model 3, as developed in section 2.3, is now applied to the food-grade CO_2 CCUS chain to identify the optimal investment timing. Three CO_2 price thresholds need to be found: $E^*_{ccs,1}$, the CO_2 price threshold to invest in CCS in Stage 1, $E^*_{ccu,2}$ and $E^*_{ccs,2}$, the CO_2 price thresholds to invest in Stage 2 in CCU and CCS, respectively.

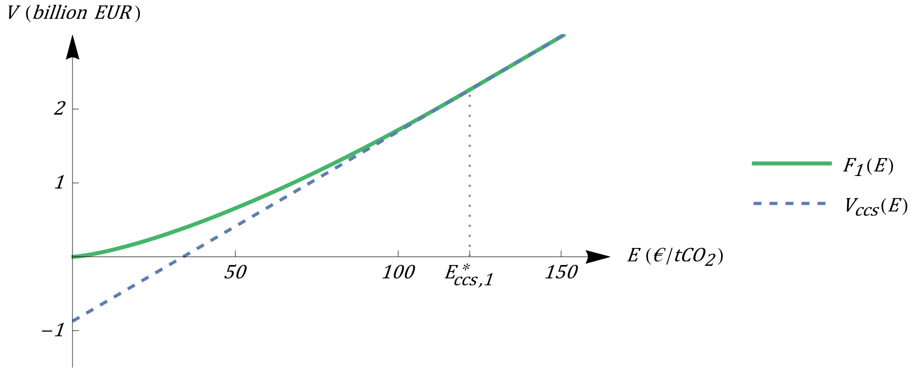
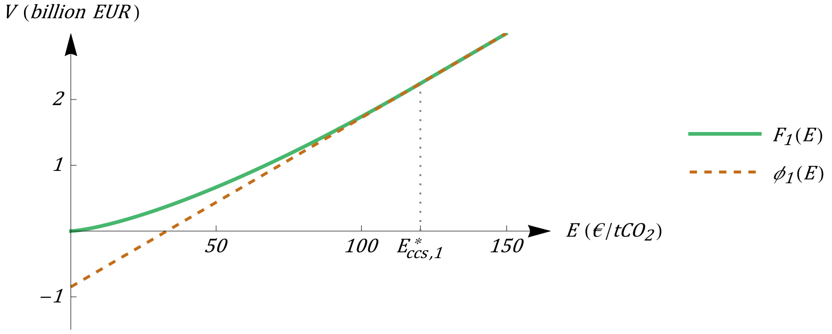


Figure 10: The option value $F_1(E)$ (green) and the present value of CCS $V_{ccs}(E)$ (blue) for the ethanol CCUS chain.

Figure 11 shows the results of Model 3 for the food-grade CO_2 CCUS chain. In Stage 1, the firm should invest in CCS once the CO_2 price exceeds 120.3 €/t CO_2. In Stage 2, the firm should invest in CCU as soon as the CO_2 price crosses 92.2 €/t CO_2. If the CO_2 price rises further and also exceeds 119.8 €/t CO_2, the firm should also adopt CCS to abate the remaining CO_2 emissions.

(a) Stage 1



(b) Stage 2

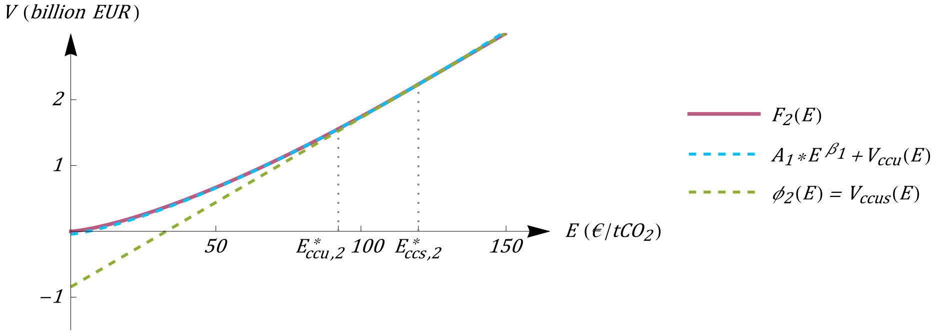


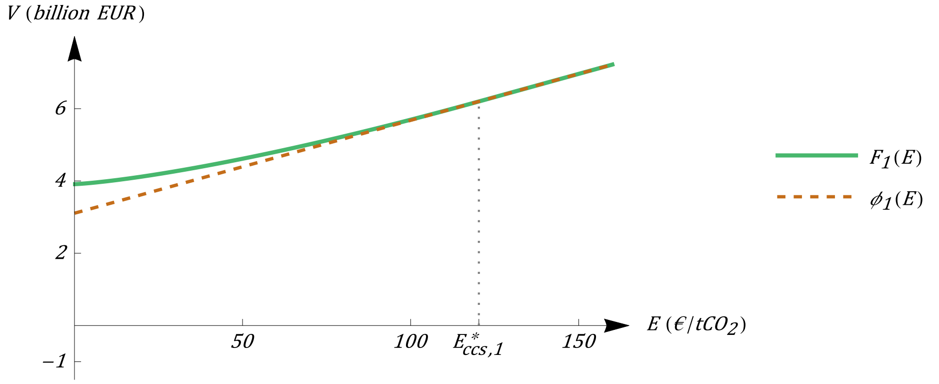
Figure 11: The option value $F_1(E)$ (green) and the present value of investing in CCS and CCU, once it arrives, $\phi_1(E)$ (dark orange) in Stage 1 and the option value $F_2(E)$ (purple), the value of having the option to invest in CCS and investing in CCU $A_1 * E^{\beta_1} + V_{ccu}(E)$ (light blue) and the present value of CCUS $V_{ccus}(E)$ (green) in Stage 2 for the food-grade CO_2 CCUS chain.

3.3 Model 4: Polyol production

Although the polyol CCUS chain involves higher investment costs I_u and higher utilization costs C_u than the food-grade CO_2 CCUS chain, it still presents a more attractive business case for CCU due to the higher product price, P_p, and higher conversion factor, X. For the polyol CCUS chain, the investment in CCU pays off, even when the CO_2 price equals zero, as can be seen in Figure 8. Hence, we can apply Model 4, as developed in Section 2.4, to the polyol CCUS chain to identify the optimal investment timing. Two CO_2 price thresholds need to be found: $E^*_{ccs,1}$ and $E^*_{ccs,2}$, the CO_2 price threshold to invest in CCS in Stage 1 and Stage 2 respectively. Figure 12 shows the results of Model 4 for the polyol CCUS chain. In Stage 1, the firm should invest in CCS once the CO_2 price exceeds 120.2 €/t CO_2. In Stage 2, the firm should adopt CCS as well, additional to CCU, when the CO_2 price crosses 119.8 €/t CO_2.

The calculated CO_2 price thresholds for each CCUS scenario are summarized in Table 3. It can be seen from Table 3 that the investment thresholds for CCS in Stage 1 for the three CCUS chains are not the same. A small decrease in the investment threshold for CCS is observed from the ethanol CCUS value chain, to the food-grade CO_2 and polyol CCUS value chain.

(*a*) *Stage 1*



(*b*) *Stage 2*

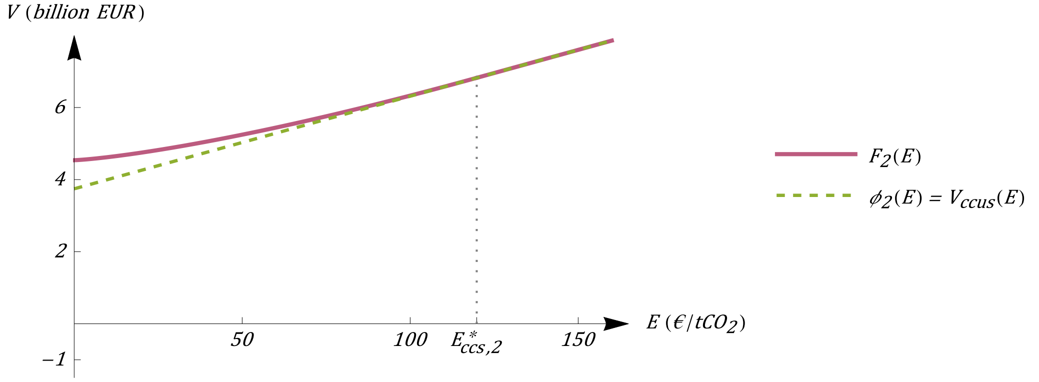


Figure 12: The option value $F_1(E)$ (green) and the present value of investing in CCS and CCU, once it arrives, $\phi_1(E)$ (dark orange) in Stage 1 and the option value $F_2(E)$ (purple) and the present value of CCUS $V_{ccus}(E)$ (green) in Stage 2 for the polyol CCUS chain.

	Ethanol	**Food-grade CO$_2$**	**Polyol**	**Unit**
$E^*_{ccs,1}$	121.9	120.3	120.2	€/t CO$_2$
$E^*_{ccu,2}$	-	92.2	-	€/t CO$_2$
$E^*_{ccs,2}$	-	119.8	119.8	€/t CO$_2$

Table 3: The CO$_2$ price thresholds in Stage 1 and Stage 2 for the three CCUS scenarios in the cement industry: ethanol production (fuel), food-grade CO$_2$ production (direct use of CO$_2$) and polyol production (chemical).

Since the costs and revenues of CCS are the same in all three CCUS chains, the discrepancy between the investment thresholds is explained by the difference in the availability and profitability of CCU. In the ethanol CCUS scenario, the arrival rate λ of the CCU solution is lower due to its lower TRL. Moreover, the CCU technology is always outperformed by the CCS technology in the ethanol CCUS scenario (Figure 8), in contrast to the food-grade CO$_2$ and polyol CCUS chain. These findings suggest that the CO$_2$ price threshold to invest in CCS is slightly reduced when the firm anticipates a more attractive CCU solution in the future (i.e. food-grade CO$_2$ and polyol), compared to when this is not anticipated (i.e. ethanol). Intuitively, one could have expected that the prospect of a more attractive abatement technology in the future, i.e. CCU, would delay investments in existing abatement technologies today, i.e. CCS. However, this observation illustrates that the anticipation of a more profitable CCU solution can stimulate early investment in CCS, or at the very least, the prospect of CCU will not counteract the investment in CCS. This can be explained by the fact that a more attractive CCU technology also makes the prospect of the CCUS value chain, as a whole, more profitable and thus, more appealing. Consequently, the firm is more eager to make the first investment to build the CCUS value chain, which explains why a more attractive future CCU technology can slightly decrease the CO$_2$ price investment threshold for CCS, even in Stage 1. Besides the differences in the investment threshold for CCS in Stage 1, it can also be seen from Table 3 how the investment threshold for CCS decreases from Stage 1 to Stage 2, for the food-grade CO$_2$ and polyol CCUS scenarios. Although the decrease is again very small, the investment in CCU, ahead of the investment in CCS, lowers the threshold to adopt CCS as well, to abate the remaining CO$_2$ emissions.

Table 4 shows the CO$_2$ price levels that should be reached to invest in CCS, CCU or CCUS in each CCUS scenario, based on a traditional NPV calculation. A comparison of Table 3 and Table 4 leads to the conclusion that the investment thresholds from the real options analysis are much higher than the CO$_2$ price levels that the firm would demand based on NPV analysis.

	Ethanol	**Food-grade CO$_2$**	**Polyol**	**Unit**
CCS	34.0	34.0	34.0	€/t CO$_2$
CCU	194.4	25.7	-2354.3	€/t CO$_2$
CCUS	38.4	32.9	-145.7	€/t CO$_2$

Table 4: The NPV CO$_2$ price levels to invest in CCS, CCU and CCUS for the three CCUS scenarios in the cement industry: ethanol production (fuel), food-grade CO$_2$ production (direct use of CO$_2$) and polyol production (chemical).

As can be seen, the inclusion of uncertainty and the flexibility to choose the timing of investments delays investments in CCS and CCU. In the next section, we will use comparative statics analysis to investigate how the CO_2 price investment thresholds respond to changes in certain parameters of the models.

4 Comparative statics

In this section, we investigate how the investment thresholds change when the level of technological uncertainty, the market uncertainty, and the cost and revenue parameters of the technologies vary. The values from the three CCUS chains in Section 3 are used as the base case values for Models 1, 3 and 4 (Table 2).

4.1 The arrival rate of CCU does not influence investment in CCS

The unknown time-to-market of CCU is the source of technological uncertainty in the model. The unknown arrival timing is characterized by the arrival rate λ, which is equivalent to an average waiting time of $1/\lambda$ years. Intuitively, the expected arrival rate could influence the optimal investment timing for CCS in the first stage.

Figure 13 shows how the investment thresholds $E^*_{ccs,1}$, $E^*_{ccu,2}$ and $E^*_{ccs,2}$ change when the arrival rate λ is varied from 0 to 1. This means that the average waiting time for CCU is varied from infinitely long to one year.

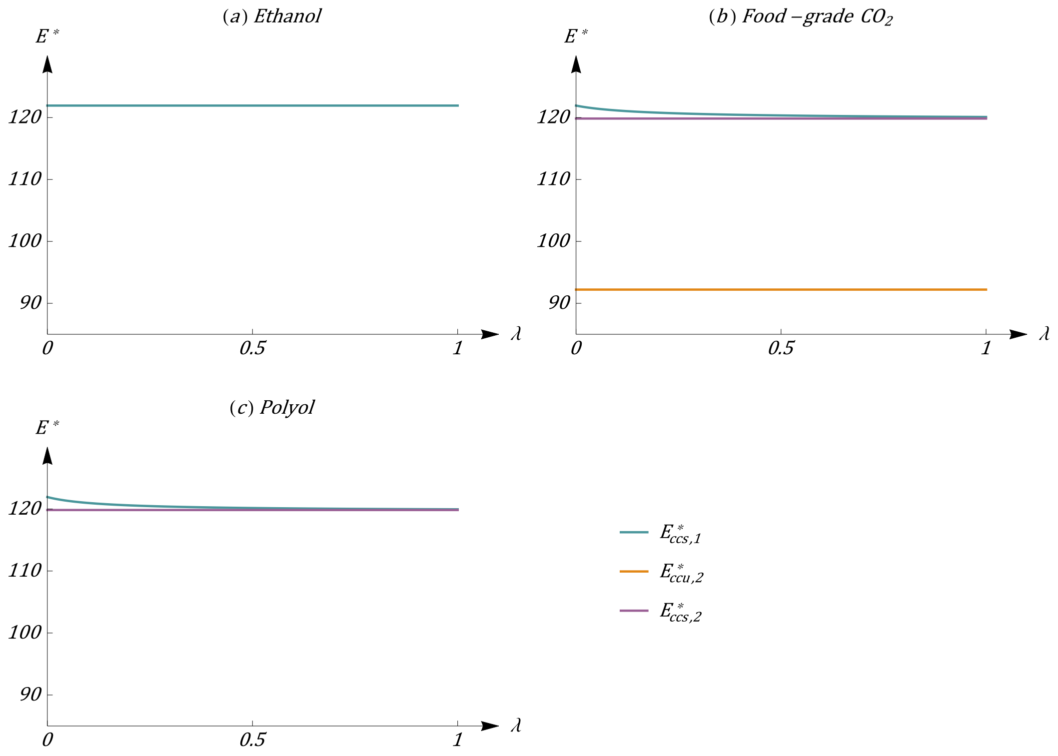


Figure 13: The influence of λ on the investment thresholds E^* for the three CCUS scenarios in Section 3.

In Stage 2, the CCU technology is mature and the uncertainty about the arrival timing is resolved. Hence, λ does not affect the investment thresholds in Stage 2 ($E^*_{ccu,2}$ and $E^*_{ccs,2}$). In Stage 1, the expected arrival of CCU could affect the incentive to invest in CCS. In Model 1, where CCS is always the optimal solution, the arrival rate of CCU does not affect the investment threshold either. In Models 3 and 4, a higher λ results in a decrease in the CCS investment threshold in Stage 1. Hence, the sooner CCU is expected, the lower the investment threshold is for CCS. However, the absolute effect of λ on the CCS investment threshold is very small, as can be seen on Figure 13. In sum, when CCU arrives - next year, in 10 years or in 100 years - barely changes the investment decision for CCS.

4.2 Volatile carbon prices delay investments

The market uncertainty is characterized by the CO_2 price, which evolves in the future according to the GBM, described in (1). The drift rate α describes the expected growth rate of the CO_2 price in each time interval and the variance parameter σ defines the standard deviation per time interval. It is valuable to analyze how variations in α and σ would affect the resulting investment thresholds.

The drift rate α is varied between 0 and 0.07, to ensure that the condition $\rho > \alpha$ remains fulfilled (Dixit and Pindyck, 1994). Figure 14 presents the influence of α on the investment thresholds in the three scenarios. This figure reveals that a higher α results in lower investment thresholds: firms are triggered to invest sooner in CCS and CCU, due to higher expected prices in the future. The effect of a higher α is similar for all models and over both stages.

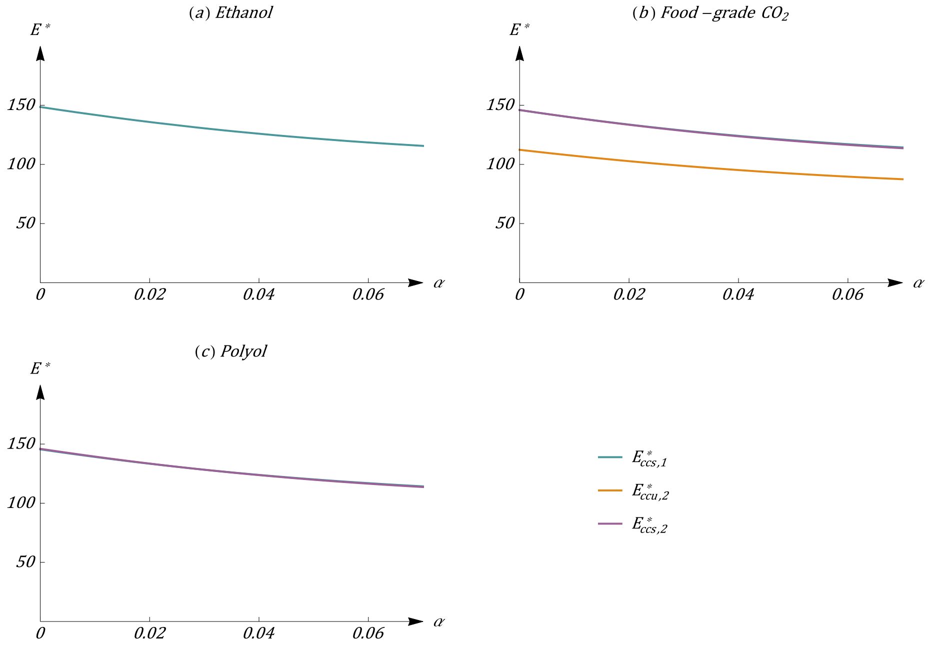


Figure 14: The influence of α on the investment thresholds E^* for the three CCUS scenarios in Section 3.

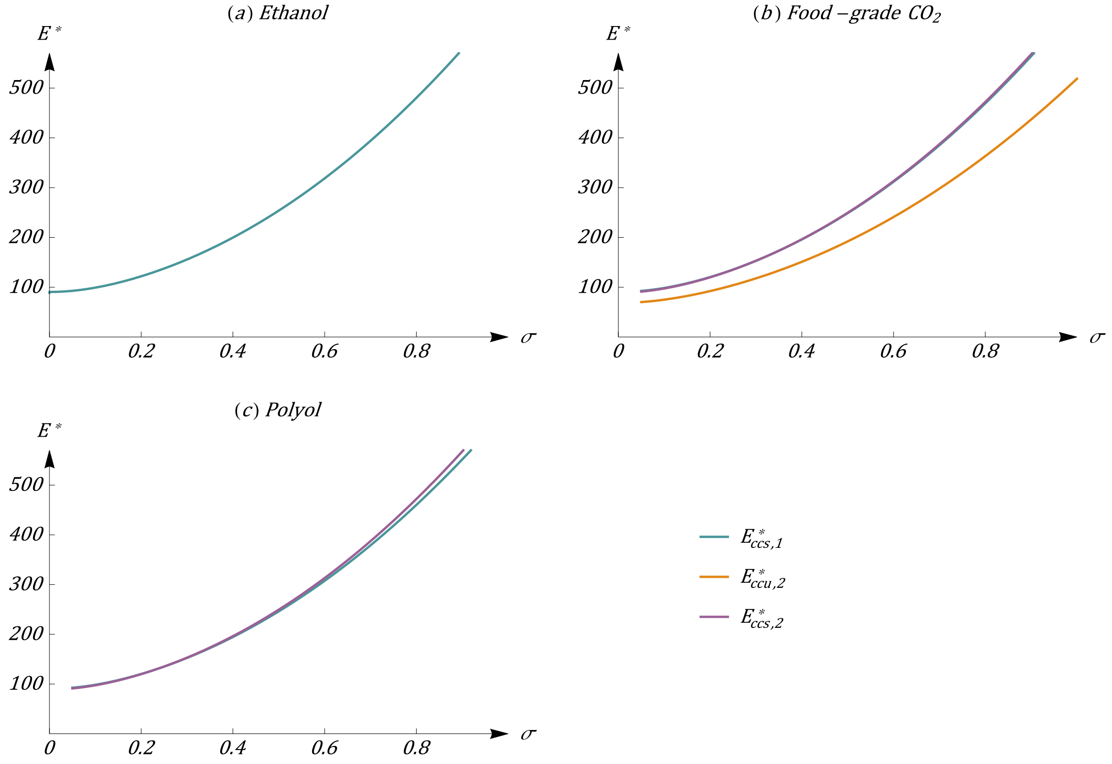


Figure 15: The influence of σ on the investment thresholds E^* for the three CCUS scenarios in Section 3.

The influence of σ on the investment thresholds is presented in Figure 15. In contrast to the growth rate α, a higher volatility σ now increases the investment thresholds. Higher uncertainty in the CO_2 price results in higher investment thresholds and thus delayed investments in CCS an CCU. This is a standard result in real options theory: the options are more valuable due to the higher uncertainty, hence, firms like to keep their options open for a longer time. This result also illustrates that uncertainty generates a value of waiting.

4.3 A higher fraction of CO_2 used stimulates investment in CCS

A crucial difference between CCS and CCU lies in the scale on which CO_2 emissions can be stored or used. The storage of CO_2 emissions can be implemented on a very large scale without running into technical or market limitations, whereas the use of CO_2 is limited to the market for the CO_2-based product. The parameter q describes the fraction of the CO_2 that can be used in the CCU route.

Figure 16 presents the influence of q on the CO_2 price thresholds to invest in CCS and CCU in the three scenarios.[3] When the investment in CCS alone is the optimal strategy, the fraction of CO_2 that can be used q does not affect the investment threshold (Figure 16 (a)).

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[3] The parameter q was varied between 0 and 1, 0.024 and 1, and 0.0006 and 1 for respectively the ethanol, food-grade CO_2 and polyol scenarios, to ensure that the conditions for each model remain fulfilled.

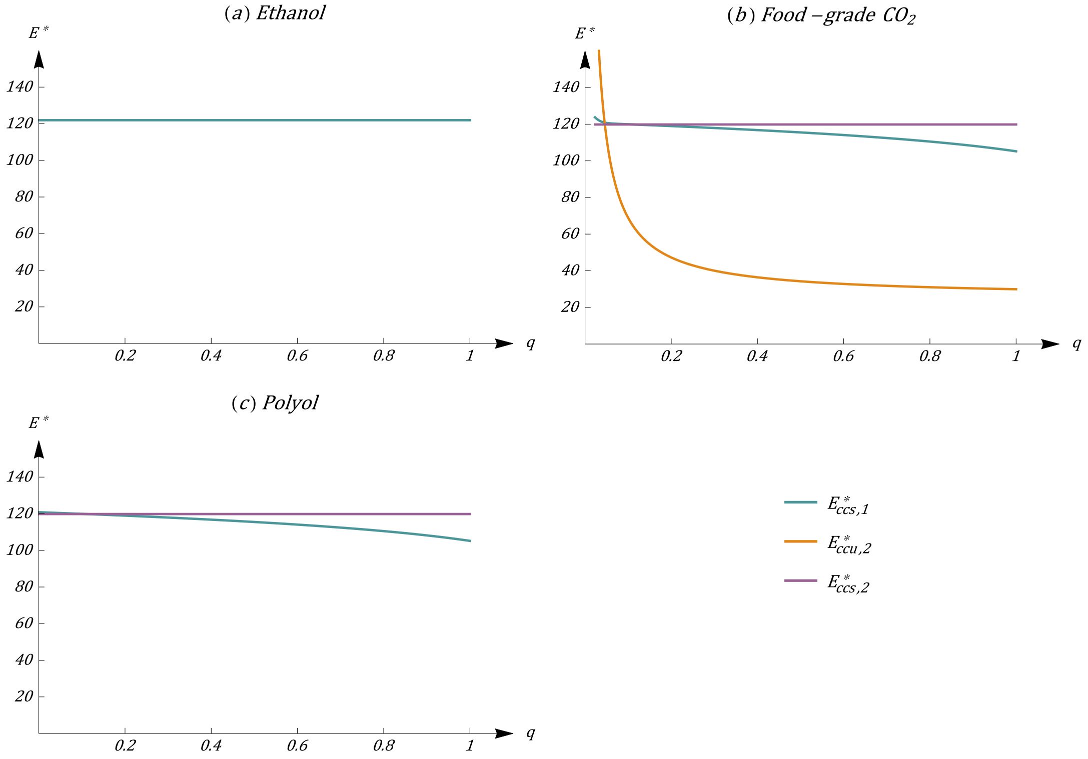


Figure 16: The influence of q on the investment thresholds E^* for the three CCUS scenarios in Section 3.

When it is optimal to invest in CCU and CCS consecutively, the fraction q clearly affects the incentive to invest in CCU: the more CO_2 can be used, the lower the CO_2 threshold to invest in CCU. The CO_2 price drops to a level below 40 €/t CO_2 for values of q higher than 0.2. Moreover, q now also influences the CO_2 price threshold to invest in CCS in the first stage (Figure 16 (b)). The influence of q on the CO_2 price threshold to invest in CCS in Stage 1 is still present when it is optimal to invest in CCU the moment it matures (Figure 16 (c)). Although the fraction of CO_2 that can be used affects the incentive to invest in CCS before CCU arrives, this effect disappears once the investment in CCU is made: the CO_2 price threshold for CCS in Stage 2 is not affected by the parameter q, both in Figure 16 (b) and (c).

The investment cost for the capture plant I_c, which needs to be incurred for both the CCS and CCU technologies, is the trigger here. When more CO_2 can be used in the CCU route, the investment cost for the capture plant is also carried more by the CCU technology. As a result, firms that anticipate the arrival of a profitable CCU technology in the future, also anticipate that the investment cost for the capture plant will be supported by the CCU route and hence, they require a lower CO_2 price to invest in CCS in Stage 1. In Stage 2, however, firms already carried out the investment for the capture plant, for the CCU route. As a result, it does not matter anymore how much CO_2 is used or stored: the investment cost I_c no longer affects the CO_2 price to invest in CCS. These intuitive explanations are confirmed by the expressions for the threshold $E^*_{ccs,2}$ (25) in Models 3 and 4, where the parameter q is not included, and for the threshold $E_{ccu,2}$ (24), where the investment costs are indeed divided by the amount of CO_2 emission that can be used.

4.4 When to invest in CCS is mostly determined by its costs

The present values of the abatement technologies over the infinite time horizon are also determined by the investment costs, operational costs, the conversion rate, and the price of the product. While changing these parameter values, we will move from one region to another in Figure 4 and the optimal adoption strategy will change. The investment costs in the capture plant, I_c, and the utilization plant, I_u, the utilization costs, C_u, the transport and storage fee, C_{ts}, the conversion rate, X and the price of the product, P_p, are all varied over the four regions in Figure 4. Figure 17 demonstrates how the investment threshold in Stage 1 $E^*_{ccs,1}$ changes when these parameters are varied over the four regions. The food-grade CO_2 CCUS chain is the starting point and is indicated by the black dot in Figure 17.

Figure 17 (a) and (b) show the influence of the investment costs I_c and the transport and storage costs C_{ts}. The investment threshold $E^*_{ccs,1}$ for CCS in Stage 1 rises when the investment cost for the capture plant I_c or the transport and storage fee C_{ts} increases. For the investment cost I_c, we observe a kink at the boundary between the light purple and dark purple region in Figure 17 (a). The effect of I_c on the threshold $E^*_{ccs,1}$ is larger in the dark purple region, where it is optimal to invest simultaneously in CCUS. Note that the cost I_c would have to become negative, to end up in the blue area. The effect of the utilization cost C_u and the investment cost for the utilization plant I_u are displayed in Figures 17 (c) and (d). The effect on $E^*_{ccs,1}$ depends on the region. When the instant CCU adoption strategy is optimal (blue), the costs C_u and I_u do not affect the threshold $E^*_{ccs,1}$. In the sequential CCU-CCS adoption strategy (light purple), at first, the threshold remains constant. However, the investment threshold $E^*_{ccs,1}$ starts to increase slightly, when we approach the next region. When the firm should invest in CCUS simultaneously (dark purple), the threshold $E^*_{ccs,1}$ increases more sharply. Nevertheless, the absolute effect remains rather small, as the threshold only varies from approximately 120 to 122 euros per tonne of CO_2. In the CCS region (red), the investment threshold again remains unchanged. Finally, Figures 17 (e) and (f) reveal the effect of the product price P_p and the conversion factor X on the threshold $E^*_{ccs,1}$. Both parameters affect the threshold $E^*_{ccs,1}$ similarly as C_u and I_u.

In sum, Figure 17 reveals that the cost parameters of the CCS technology, i.e. I_c and C_{ts}, affect the threshold to invest in CCS in Stage 1 the most. The parameters that are specific to the CCU technology, i.e. C_u, I_u, P_p and X, only affect the CO_2 price threshold to invest in CCS in Stage 1 minimally. Figures 17 (c) - (e) show that the CO_2 price only varies between 120 and 122 €/t CO_2.

In Figure 17, we adjust the selected adoption strategy to the changed parameter assumptions. Figure A.5 demonstrates how the threshold would change when we would not change the adoption strategy and only consider one adoption strategy. When the conversion rate X is varied between 0 and 1, we can now observe that the CO_2 price threshold to invest in CCS changes from 145 €/t CO_2 to 120 €/t CO_2. We conclude that adjusting the chosen adoption strategy to changing circumstances, helps to flatten out the effect on the investment threshold.

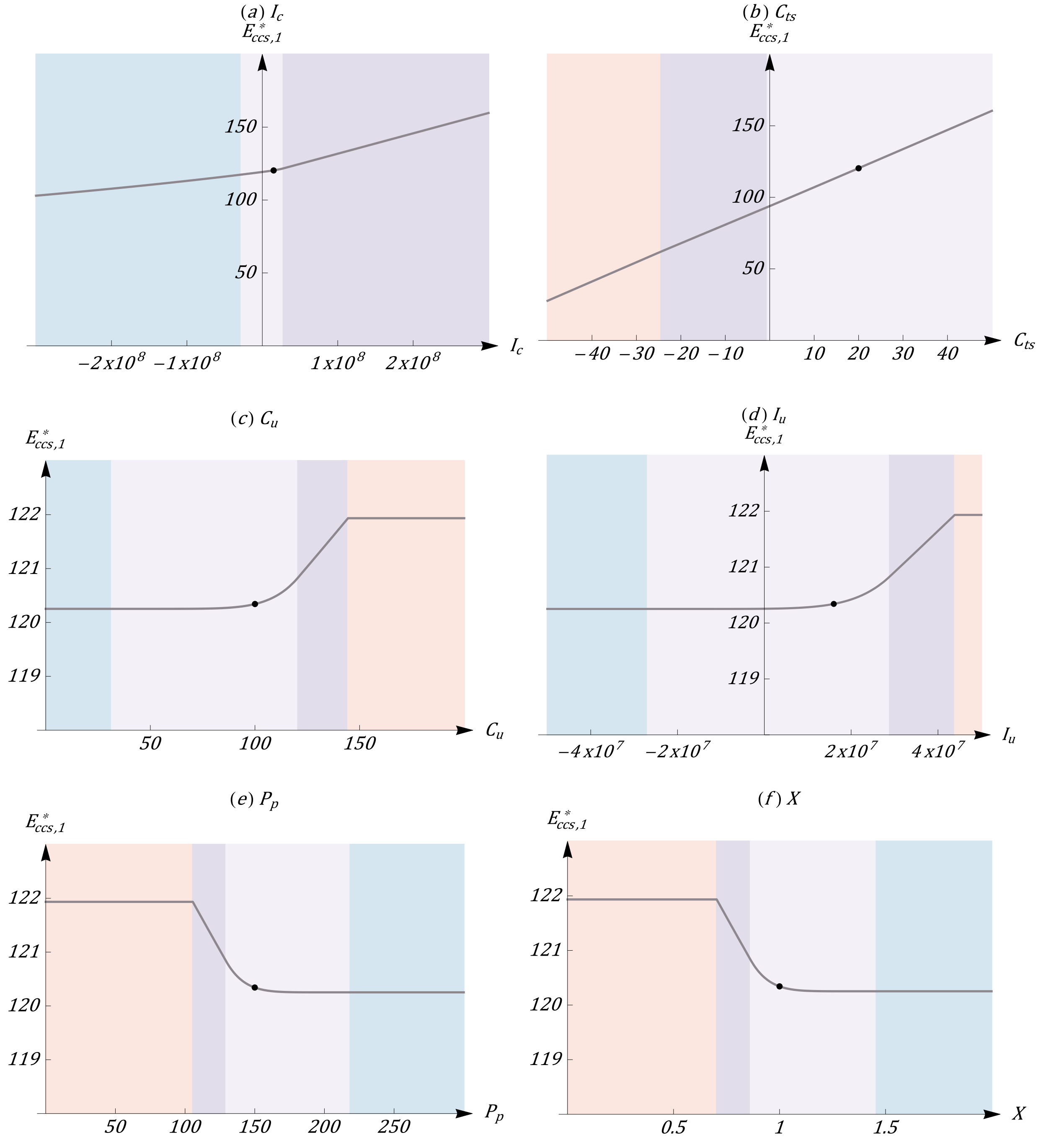


Figure 17: The influence of (a) I_c, (b) C_{ts}, (c) C_u, (d) I_u, (e) P_p and (f) X on the investment thresholds $E^*_{ccs,1}$. The red, dark purple, light purple, and blue areas reflect the optimal regions for respectively the CCS, simultaneous CCUS, sequential CCU-CCS, and instant CCU adoption strategy. The black dots represent the base case, i.e. the food-grade CO_2 (Table 2).

5 Discussion

Our work demonstrates the need to develop four different real options models to accommodate the different adoption strategies that are optimal under different conditions. Grenadier and Weiss (1997) paved the way by identifying four different adoption strategies when a firm is confronted with a sequence of two technological innovations. We build on their work by not only allowing one technological innovation to replace the other but also allowing the co-existence of both innovations. While Grenadier and Weiss (1997) found that slow innovation (i.e. low λ) resulted in earlier adoption of the existing technology, we observe the effect of the innovation pace λ on the investment in the existing technology (CCS) to be minimal. In contrast to the findings of Grenadier and Weiss (1997), the more attractive the future innovation (CCU) is, the sooner the firm will adopt the existing innovation (CCS). This difference in findings can be explained by the fact that in the current study, the new technological innovation does not necessarily replace the existing technology but can complement and improve its performance.

The potential of coupling CCS and CCU was indeed investigated explicitly in this study. Whether CCU and CCS are complementary or competitive solutions has been debated before in literature. While some argue that CCU can serve as a stepping stone towards CCS, by valorizing the captured CO_2 and reducing the high costs associated with CCS (Ampelli et al., 2015; Hepburn et al., 2019), others claim that CCU will not be able to reduce the costs of CCS and that it will only distract the attention from CCS, because of the limited scale on which CCU can be implemented (Mac Dowell et al., 2017). Within the theoretical framework of the developed real options models, we find that having the possibility to invest in CCU in the future does not reduce the willingness to invest in CCS today. On the contrary, we observed that the CO_2 price threshold to invest in CCS was lowered when the firms anticipated the arrival of a profitable CCU technology in the route. In this study, the limitations of the scale of CCU were taken into account. Previous studies also analyzed the role of CO_2-EOR as a driver to stimulate the deployment of large-scale CCS (Santos et al., 2021; Kolster et al., 2017). These studies demonstrated how the linkage of CO_2-EOR and CCS can make CCS more attractive as well. However, the scale of CO_2-EOR is much larger than the scale of CCU routes considered in this study.

Another important finding was that higher volatility of the CO_2 price in the EU ETS, described by σ, resulted in delayed investments in CCS. This finding is consistent with that of Compernolle et al. (2017) and Lin and Tan (2021), who found that higher CO_2 price uncertainty resulted in higher investment thresholds. This highlights the need for EU policymakers to provide a stable framework for the EU ETS. A study on the behavior of the carbon price in the EU ETS demonstrated how a steep increase in the volatility of the carbon price is expected by the end of a trading period (Seifert et al., 2008). Combined with the results of our real options analysis, this implies that firms will postpone their investments in carbon abatement solutions further as the end of the next trading period (2030) approaches. Hence, it is crucial that policymakers are transparent and try to smooth the transition from one trading period to another, to lower the expected volatility in the carbon price.

In this study, we considered the possibility of combining both CCS and CCU in one value chain, to mitigate all CO_2 emissions of one plant. Hence, we implicitly assumed that all CO_2 emissions used in the CCU route are also accounted as not-emitted in the EU ETS. In practice, only CO_2 emissions that are captured and then (1) transported for permanent storage or (2) that have been utilized in such a way that they are permanently chemically bound are exempted from paying emission allowances (EC, 2023b). In the future, the EU ETS may include a broader regulatory framework for CCU. However, the EU ETS will probably not consider all captured and used CO_2 emissions directly as not-emitted but will require detailed life cycle assessments to calculate how much CO_2 is really avoided. Further work is needed to evaluate how different regulations for utilized CO_2 in the EU ETS would affect the investment decision in CCU.

One of the other underlying assumptions of the real options model was that one actor invests in and operates both the CO_2 capture and the CO_2 utilization plant. Another approach would be that the firm 'outsources' the CO_2 utilization, similar to the outsourcing of the transport and storage of CO_2 in the CCS value chain. In this case, the firm captures the CO_2 itself but then sells the CO_2 at a certain price to another firm that can utilize the CO_2. In this approach, the price that the CO_2-emitting firm receives is likely to be dependent on the utilization cost per tonne of CO_2 (C_u), the investment for the utilization plant (I_u) and the product price (P_P) that the other firm would incur. Hence, including these variables directly in our model can be seen as a vertical integration of the CO_2-emitting and the CO_2-utilizing firm. Moreover, the assumption that the CO_2-emitter could sell its CO_2 to another firm that can utilize the CO_2, would be contingent on the existence of a market for CO_2, where CO_2 can actually be traded physically between firms, and probably across borders. Examples of cross-border trade of CO_2 are emerging only recently and can to date only be found for the transport and storage of CO_2. For example, in March 2023, the Greensand project was inaugurated, which involves the capture and shipping of $CO2_2$ from Belgium to a depleted oil field in Denmark, where the CO_2 can be stored. This project is currently still in a pilot phase. In sum, the (cross-border) trade of CO_2 for $CO2_2$ utilization would first require the development of a regulatory framework and the required infrastructure for CO_2 transport. Therefore, the assumption was made that the utilization of CO_2 is performed on-site, by the same actor, eliminating the need for CO_2 transport in the CCU value chain and the regulatory uncertainty that would be associated with this. However, future research could investigate how the 'outsourcing' of CO_2 utilization as a business model would affect the results of the real options analysis.

Further research is also needed to establish the environmental implications of the findings of this study. The results indicated that firms delay their investments in CCS or CCU when they are confronted with uncertainty about the carbon price and when they have the flexibility to postpone their investment decision. An implication of this is that the abatement of CO_2 emissions is postponed, which is not desirable from the societal perspective. As indicated by previous research, early action to mitigate climate change is needed, also to contain the cost of mitigation (Bosetti et al., 2012). This is an important issue for future research. Therefore, a future study that includes the environmental impact (and cost) of the delayed abatement of CO_2 emissions is suggested. Combining both economic and environmental perspectives into the real options analysis is an interesting and challenging issue for future research.

6 Conclusion

In this study, we show how to tackle the technological and market uncertainties that are present while making investment decisions for CCS and CCU technologies. Moreover, the possibility to combine CCS and CCU in an integrated CCUS installation is investigated as well. To do so, we develop a real options model that determines the optimal timing to invest in CCS and CCU, while taking into account the unknown arrival of CCU and the CO_2 price uncertainty. The real options analysis reveals three main findings. First, the presence of technological and market uncertainties, accounted for in the real options model, increase the barriers to invest in CCS or CCU. Second, when the firm anticipates the arrival of a more attractive CCU solution in the future, it will not postpone the investment in CCS. On the contrary, the CO_2 price threshold to invest in CCS is slightly lowered when the firm expects a profitable CCU technology in the future. Whether this new CCU technology arrives next year or only in ten years, does not affect the investment threshold for CCS to a great extent. Third, higher uncertainty in the CO_2 price, i.e. higher σ, increases the investment thresholds, while a higher trend in the CO_2 price, i.e. higher α, decreases the investment thresholds for CCS and CCU. Hence, this study confirms the observation from previous papers (Compernolle et al., 2017; Lin and Tan, 2021) that higher uncertainty in the CO_2 price delays the investment in CCS or CCU.

This study generates useful insights, both for firms that want to invest in CCUS technologies and for policymakers that want to reduce the barriers to invest in these solutions. Firms that aim to optimize their investments in CO_2 abatement technologies should consider the flexibility and market and technological uncertainty present in their investment decision. Otherwise, firms will invest too early, i.e. at too low CO_2 price levels. Moreover, firms should make efforts to investigate how profitable the CCU technology in the future will be. The more attractive the CCU technology is, the lower the investment threshold for CCS is today. From the policymaker's perspective, three recommendations can be formulated based on the results. First, policymakers should aim to ensure stability and predictability in the CO_2 price, to lower the volatility σ of the CO_2 price. Reducing the market uncertainty will lower the CO_2 price investment thresholds for CCS, CCU and CCUS. Second, they should also commit to an increasing growth rate in the CO_2 price in the EU ETS. When firms expect higher growth rates for the CO_2 price in the future, they are more favourable to invest in CCS, CCU and CCUS sooner. Finally, policymakers should realize that CCU and CCS can be complementary solutions. We find that the anticipation of more profitable CCU technologies in the future did not delay investments in CCS today. Firms will even invest in CCS at slightly lower CO_2 prices today and hence, initiate the abatement of CO_2 emissions sooner.

A Appendix

A.1 Model 1

The general solution for the ODE in (7) yields $F_1(E) = A_1 \cdot E^{\beta_1} + A_2 \cdot E^{\beta_2}$, where β_1 and β_2 are respectively the positive and negative roots of the quadratic equation $\frac{1}{2}\sigma^2\beta^2 + (\alpha - \frac{1}{2}\sigma)\beta - \rho = 0$, and A_1 and A_2 are constants that remain to be determined. If the CO_2 price equals zero, it will remain zero according to expression (1), and, since then there is no reason for the firm to abate, the option value should equal zero as well. Since $F_1(0) = 0$ and $\beta_2 < 0$, it follows that $A_2 = 0$ (otherwise, $F_1(0) \to \infty$). Hence, the value of the option in the waiting region equals

$$F_1(E) = A_1 \cdot E^{\beta_1}, \quad with \tag{A.1}$$

$$\beta_1 = \frac{-\alpha + \frac{1}{2} \cdot \sigma^2 + \sqrt{(\alpha - \frac{1}{2} \cdot \sigma^2)^2 + 2 * \sigma^2 * \rho}}{\sigma^2}. \tag{A.2}$$

Combining the expected present value of operating CCS (5) and the value of waiting (A.1) yields the expression for $F_1(E)$:

$$F_1(E) = \begin{cases} A_1 \cdot E^{\beta_1} \quad \text{if} \quad E \leq E^*_{ccs}, \\ \frac{Q_{co_2}}{\rho-\alpha} \cdot E - \frac{Q_{co_2}}{\rho} \cdot (C_c + C_{ts}) - I_c \quad \text{if} \quad E > E^*_{ccs}. \end{cases} \tag{A.3}$$

When the CO_2 price equals the investment threshold E^*_{ccs}, the firm is indifferent between investing and waiting. Following Dixit and Pindyck (1994), the optimal investment threshold E^*_{ccs} and the constant A_1 are now determined analytically by applying value-matching and smooth-pasting conditions to the two branches of (A.3). These conditions are indicated in (A.4) and (A.5):

$$A_1 \cdot (E^*_{ccs})^{\beta_1} = \frac{Q_{co_2}}{\rho - \alpha} \cdot E^*_{ccs} - \frac{Q_{co_2}}{\rho} \cdot (C_c + C_{ts}) - I_c, \tag{A.4}$$

$$A_1 \cdot \beta_1 \cdot (E^*_{ccs})^{\beta_1 - 1} = \frac{Q_{co_2}}{\rho - \alpha}. \tag{A.5}$$

The value matching condition in (A.4) simply states that at the threshold, the value of waiting (left-hand side) should equal the value of the investment (right-hand side). The smooth pasting condition in (A.5) stipulates that the slope of both curves should also be equal at the threshold. Solving this system of equations yields a solution for E^*_{ccs} and A_1, as presented in equations (9) and (10). Figure A.1 summarizes the investment decision for the firm in Model 1.

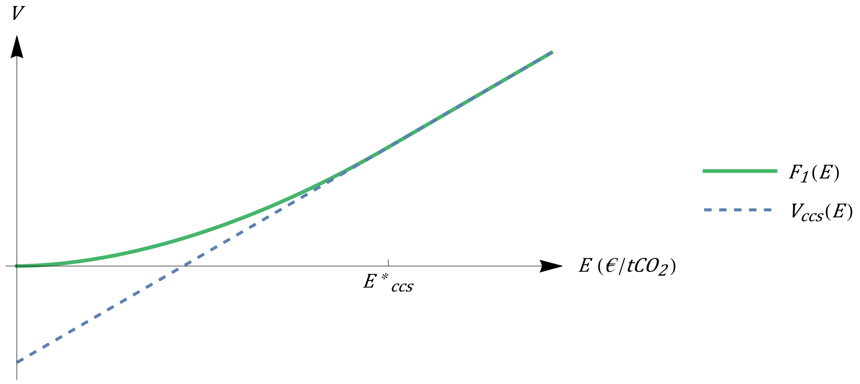


Figure A.1: The firm's investment decision problem, in Model 1.

A.2 Model 2

Model 2 finds the optimal timing to invest in CCS in Stage 1 and in CCUS in Stage 2, when the optimal strategy is to invest simultaneously in CCUS.

A.2.1 Stage 2

The value of the option to invest in CCUS is given by

$$F_2(E) = A_1 \cdot E^{\beta_1}. \tag{A.6}$$

Combining the expressions for $F_2(E)$ in the stopping region, i.e. the expected present value of operating CCUS (11), and in the waiting region, i.e. (A.6), characterizes $F_2(E)$ for all E:

$$F_2(E) = \begin{cases} A_{1,sim} \cdot E^{\beta_1} \quad \text{if} \quad E \leq E^*_{ccus}, \\ \frac{Q_{co_2}}{\rho-\alpha} \cdot E - \frac{Q_{co_2}}{\rho} \cdot C_c - \frac{(1-q)*Q_{co_2}}{\rho} \cdot C_{ts} + \frac{q*Q_{co_2}}{\rho} \cdot (P_p \cdot X - C_u) - I_c - I_u \quad \text{if} \quad E > E^*_{ccus}. \end{cases} \tag{A.7}$$

The solution for $F_2(E)$ is indicated in (A.7), where the threshold $E^*_{ccus,2}$ and the constant $B_{1,sim}$ are obtained analytically via the value matching and smooth pasting conditions in (A.8) and (A.9):

$$B_{1,sim}(E^*_{ccus})^{\beta_1} = \frac{Q_{co_2}}{\rho-\alpha}E^*_{ccus} - \frac{Q_{co_2}}{\rho}CC - \frac{(1-q)Q_{co_2}}{\rho} \cdot C_{ts} + \frac{q \cdot Q_{co_2}}{\rho}(P_p \cdot X - C_u) - I_c - I_u, \tag{A.8}$$

$$B_{1,sim}(E^*_{ccus})^{\beta_1-1} = \frac{Q_{co_2}}{\rho-\alpha}. \tag{A.9}$$

A.2.2 Stage 1

The dynamics of $F_1(E)$ were described in (17). Applying Ito's Lemma to find the derivative of $F_1(E)$ results in

$$dF_1 = \alpha E F_1^{'} dt + \frac{1}{2}\sigma^2 * E^2 * F_1^{"} dt + \sigma E F_2^{'} dz + \lambda(F_2 - F_1)dt. \tag{A.10}$$

The resulting ODE is indicated in (18). Note that the solution of the homogeneous part $(\frac{1}{2}\sigma^2 E^2 F_1^{"}(E) + \alpha E F_1'(E) - (\rho+\lambda)F_1(E))$ is $F_1(E) = C_1 \cdot E^{\delta_1} + C_2 \cdot E^{\delta_2}$. Since $F_1(0) = 0$ and $\delta_2 < 0$, C_2 should again be equal to zero (otherwise, $F_1(0) \to \infty$). The particular solution is based on $F_2(E)$, adjusted by the term λ because CCU has yet to become available. The value matching and smooth pasting conditions at $E^*_{ccus,2}$ are indicated in (A.11) and (A.12).

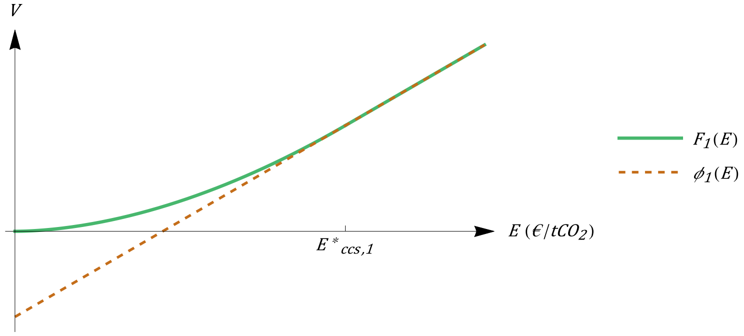
$$\begin{aligned} B_1(E^*_{ccus,2})^{\delta_1} + A_{1,sim}(E^*_{ccus,2})^{\beta_1} &= B_4(E^*_{ccus,2})^{\delta_2} + \frac{\lambda}{\lambda+\rho-\alpha}\frac{Q_{co_2}}{\rho-\alpha}E^*_{ccus,2} + \\ \frac{\lambda}{\lambda+\rho} * \left[-\frac{Q_{co_2}}{\rho} \cdot C_c - \frac{(1-q) \cdot Q_{co_2}}{\rho} * C_{ts} + \frac{q \cdot Q_{co_2}}{\rho} * (P_p * X - C_u) - I_c - I_u \right]&, \end{aligned} \tag{A.11}$$

$$B_1(E^*_{ccus,2})^{\delta_1-1} + A_{1,sim}(E^*_{ccus,2})^{\beta_1-1} = B_4(E^*_{ccus,2})^{\delta_2-1} + \frac{\lambda}{\lambda+\rho-\alpha}\frac{Q}{\rho-\alpha}. \tag{A.12}$$

Solving this system of equations results in the solution for B_1, B_4, and $E^*_{ccus,2}$ (14).

Figure A.2 illustrates the value functions for the firm in Model 2. Figure A.2(a) shows how $F_1(E)$ and $\phi_1(E)$ match at the investment threshold $E^*_{ccs,1}$ in Stage 1. Similarly, in Stage 2, $F_2(E)$ and the value from operating CCUS (adjusted for its unknown arrival) converge at the investment threshold $E^*_{ccus,2}$.

(a) Stage 1



(b) Stage 2

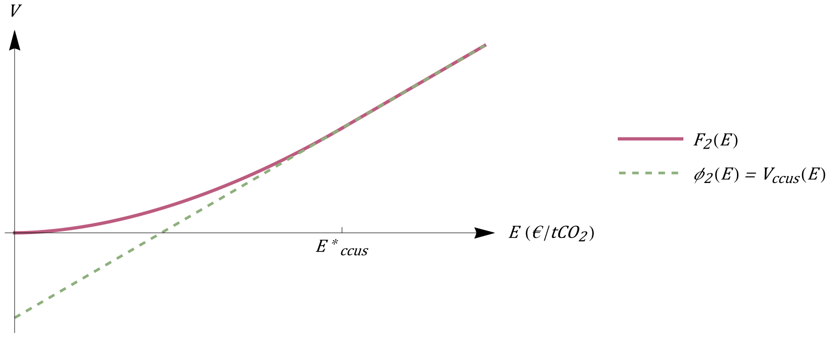


Figure A.2: The firm's investment decision problem in Stage 1 and Stage 2, in Model 2.

A.3 Model 3

Model 3 finds the optimal timing to invest in CCS in Stage 1 and in CCU and CCS in Stage 2, when the optimal strategy is to invest sequentially in CCU and CCS.

A.3.1 Stage 2

The solution for $F_2(E)$ is indicated in (23). The thresholds $E^*_{ccu,2}$ and $E^*_{ccs,2}$ and the constants $A_{1,seq}$ and D_1 are determined analytically via the value-matching and smooth pasting conditions in (A.13), (A.14), (A.15) and (A.16).

$$A_{1,seq} \cdot \left(E^*_{ccu,2}\right)^{\beta_1} = D_1 \cdot \left(E^*_{ccu,2}\right)^{\beta_1} + \frac{q \cdot Q}{\rho - \alpha} * E^*_{ccu,2} + \frac{q \cdot Q_{co_2}}{\rho} * (P_p * X - C_c - C_u) - I_c - I_u, \tag{A.13}$$

$$A_{1,seq} \cdot \beta_1 \cdot \left(E^*_{ccu,2}\right)^{\beta_1 - 1} = D_1 \cdot \beta_1 \cdot \left(E^*_{ccu,2}\right)^{\beta_1 - 1} + \frac{q \cdot Q_{co_2}}{\rho - \alpha}, \tag{A.14}$$

$$\begin{gathered} D_1 \cdot \left(E^*_{ccs,2}\right)^{\beta_1} + \frac{q \cdot Q_{co_2}}{\rho - \alpha} * E^*_{ccs,2} + \frac{q \cdot Q_{co_2}}{\rho} * (P_p * X - C_c - C_u) - I_c - I_u = \\ \frac{Q_{co_2}}{\rho - \alpha} E^*_{ccs,2} - \frac{Q_{co_2}}{\rho} \cdot C_c - \frac{(1-q) Q_{co_2}}{\rho} C_{ts} + \frac{q \cdot Q_{co_2}}{\rho} (P_p \cdot X - C_u) - I_c - I_u, \end{gathered} \tag{A.15}$$

$$D_1 \cdot \left(E^*_{ccs,2}\right)^{\beta_1} + \frac{q * Q_{co_2}}{\rho - \alpha} = \frac{Q_{co_2}}{\rho - \alpha}. \tag{A.16}$$

The solutions for the constants $A_{1,seq}$ and D_1 are given by:

$$A_{1,seq} = D_1 + \frac{q \cdot Q_{co_2}}{\rho - \alpha} \cdot \frac{1}{\beta_1} \cdot \left[\frac{\beta_1}{\beta_1 - 1} \cdot \left(\frac{\rho - \alpha}{\rho} \cdot (C_c + C_u - P_p \cdot X) + \frac{\rho - \alpha}{q \cdot Q_{co_2} Q} \cdot (I_c + I_u)\right)\right]^{1-\beta_1}, \tag{A.17}$$

$$D_1 = \frac{(1-q)Q}{\rho - \alpha} \cdot \frac{1}{\beta_1} \cdot \left[\frac{\beta_1}{\beta_1 - 1} \cdot \frac{\rho - \alpha}{\rho} \cdot (C_c + C_{ts})\right]^{1-\beta_1}. \tag{A.18}$$

A.3.2 Stage 1

The dynamics of $F_1(E)$ were described in (17). Applying Ito's Lemma to find the derivative of $F_1(E)$ results in

$$dF_1 = \alpha * E * F_1^{'} dt + \frac{1}{2} * \sigma^2 * E^2 * F_1^{''} dt + \sigma * E * F_2^{'} dz + \lambda(F_2 - F_1)dt. \tag{A.19}$$

The resulting ODE is indicated in (18). Note that the solution of the homogeneous part ($\frac{1}{2}\sigma^2 E^2 F_1''(E) + \alpha E F_1'(E) - (\rho + \lambda)F_1(E)$) is $F_1(E) = C_1 \cdot E^{\delta_1} + C_2 \cdot E^{\delta_2}$. Since $F_1(0) = 0$ and $\delta_2 < 0$, C_2 should again be equal to zero (otherwise, $F_1(0) \to \infty$). The particular solution is based on $F_2(E)$, adjusted by the term λ because CCU has yet to become available. The value-matching and smooth pasting conditions at respectively $E^*_{ccu,2}$ and $E_{ccs,2}$ are indicated in (A.20) - (A.23).

$$\begin{aligned}
&A_{1,seq} \cdot \left(E^*_{ccu,2}\right)^{\beta_1} + B_{1,seq} \cdot \left(E^*_{ccu,2}\right)^{\delta_1} = \frac{\lambda}{\rho + \lambda - \alpha} \cdot \frac{q * Q}{\rho - \alpha} \cdot E^*_{ccu,2} + \\
&\frac{\lambda}{\lambda + \rho} \cdot \left[\frac{q \cdot Q_{co_2}}{\rho} \cdot (P * X - C_u - C_c) - I_c - I_u\right] + D_1 \cdot \left(E^*_{ccu,2}\right)^{\beta_1} + B_{2,seq} \cdot \left(E^*_{ccu,2}\right)^{\delta_1} + B_{3,seq} \cdot \left(E^*_{ccu,2}\right)^{\delta_2},
\end{aligned} \tag{A.20}$$

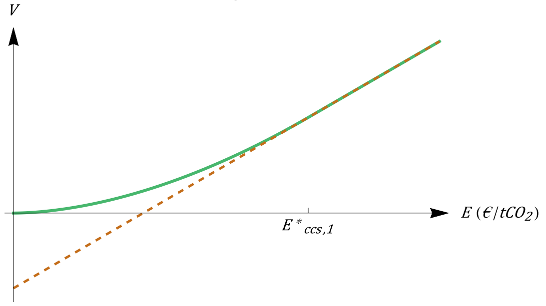
$$\begin{aligned}
&A_{1,seq} \cdot \beta_1 \cdot \left(E^*_{ccu,2}\right)^{\beta_1 - 1} + B_{1,seq} \cdot \delta_1 \cdot \left(E^*_{ccu,2}\right)^{\delta_1 - 1} = \frac{\lambda}{\rho + \lambda - \alpha} \cdot \frac{q \cdot Q_{co_2}}{\rho - \alpha} + D_1 \cdot \beta_1 \cdot \left(E^*_{ccu,2}\right)^{\beta_1 - 1} + \\
&B_{2,seq} \cdot \delta_1 \cdot \left(E^*_{ccu,2}\right)^{\delta_1 - 1} + B_{3,seq} \cdot \delta_2 \cdot \left(E^*_{ccu,2}\right)^{\delta_2 - 1},
\end{aligned} \tag{A.21}$$

$$\begin{aligned}
&\frac{\lambda}{\rho + \lambda - \alpha} \cdot \frac{q * Q_{co_2}}{\rho - \alpha} \cdot E^*_{ccs,2} + \frac{\lambda}{\lambda + \rho} \cdot \left[\frac{q * Q_{co_2}}{\rho} \cdot (P_p * X - C_u - C_c) - I_c - I_u\right] + D_1 \cdot \left(E^*_{ccs,2}\right)^{\beta_1} + \\
&B_{2,seq} \cdot \left(E^*_{ccs,2}\right)^{\delta_1} + B_{3,seq} \cdot \left(E^*_{ccs,2}\right)^{\delta_2} = \frac{\lambda}{\rho + \lambda - \alpha} * \frac{q * Q_{co_2}}{\rho - \alpha} \cdot E^*_{ccs,2} + \frac{\lambda}{\lambda + \rho} * \Big[-\frac{Q}{\rho} * CC - (1-q) \cdot Q_{co_2} \cdot C_{ts} + \\
&\frac{q \cdot Q_{co_2}}{\rho} * (P_p \cdot X - C_i) - I_c - I_u\Big] + B_{4,seq} * \left(E^*_{ccs,2}\right)^{\delta_2},
\end{aligned} \tag{A.22}$$

$$\begin{aligned}
&\frac{\lambda}{\rho + \lambda - \alpha} \cdot \frac{q * Q_{co_2}}{\rho - \alpha} \cdot + D_1 \cdot \beta_1 \cdot \left(E^*_{ccs,2}\right)^{\beta_1 - 1} + B_{2,seq} \cdot \delta_1 \cdot \left(E^*_{ccs,2}\right)^{\delta_1 - 1} + B_{3,seq} \cdot \delta_2 \cdot \left(E^*_{ccs,2}\right)^{\delta_2 - 1} = \\
&\frac{\lambda}{\rho + \lambda - \alpha} * \frac{q * Q_{co_2}}{\rho - \alpha} \cdot E^*_{ccs,2} + \frac{\lambda}{\lambda + \rho} * \big[-\frac{Q}{\rho} * C_c - (1-q) * Q_{co_2} * C_{ts} + \frac{q * Q_{co_2}}{\rho} * (P_p * X - C_u) - I_c - I_u\big] + \\
&B_{4,seq} \cdot \delta_2 \cdot \left(E^*_{ccs,2}\right)^{\delta_2 - 1}.
\end{aligned} \tag{A.23}$$

Figure A.3 summarizes the investment decision for the firm in Model 3. Figure A.3 (a) shows how $F_1(E)$ and $\phi_1(E)$ match at the investment threshold $E_{ccs,1}$ in Stage 1. Figure A.3 (b) illustrates the threefold character of $F_2(E)$. At $E^*_{ccu,2}$, the value function $F_2(E)$ aligns with the expected profits of CCU and the option to invest in CCS (blue dashed line). When the CO_2 price rises further until $E^*_{ccs,2}$, the value function $F_2(E)$ collapses with the profits of CCUS (green dashed line).

(a) Stage 1



(b) Stage 2

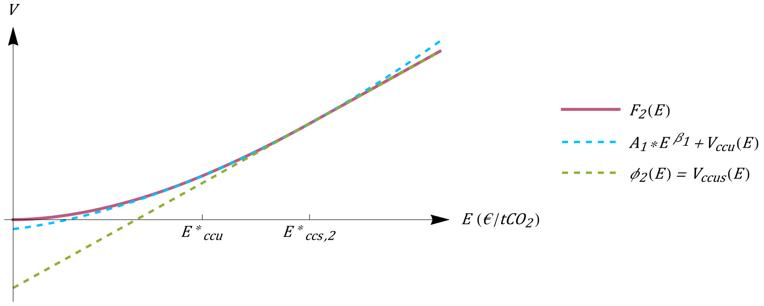


Figure A.3: The firm's investment decision problem in Stage 1 and Stage 2, in Model 3.

A.4 Model 4

Model 4 finds the optimal timing to invest in CCS in Stage 1 and in CCS in Stage 2, when the optimal strategy is to invest immediately in CCU when it arrives, followed by CCS later.

A.4.1 Stage 1

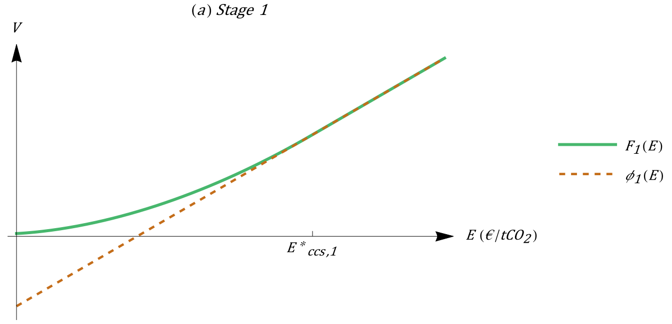
The value-matching and smooth pasting conditions at $E^*_{ccs,1}$ are indicated in (A.24) - (A.25).

$$\begin{aligned}
&A_{1,imm} \cdot \left(E^*_{ccus,2}\right)^{\beta_1} + \frac{\lambda}{\lambda+\rho-\alpha}\frac{q\cdot Q_{co_2}}{\rho-\alpha}E^*_{ccus,2} + \frac{\lambda}{\lambda+\rho} + \frac{q\cdot Q_{co_2}}{\rho}\left[(P_p\cdot X - C_c - C_u) - I_c - I_u\right] + B_{1,imm} * \left(E^*_{ccus,2}\right)^{\delta_1} \\
&= \frac{\lambda}{\lambda+\rho-\alpha}\frac{Q_{co_2}}{\rho-\alpha} * E^*_{ccus,2} + \frac{\lambda}{\lambda+\rho}\left[-\frac{Q_{co_2}}{\rho} * C_c - \frac{(1-q)\cdot Q_{co_2}}{\rho} * C_{ts} + \frac{q\cdot Q_{co_2}}{\rho}\cdot(P_p\cdot X - C_u) - I_c - I_u\right] \\
&+ B_{4,imm} * \left(E^*_{ccus,2}\right)^{\delta_2},
\end{aligned} \tag{A.24}$$

$$\begin{aligned}&A_{1,imm} \cdot \beta_1 \cdot \left(E^*_{ccus,2}\right)^{\beta_1 - 1} + \frac{\lambda}{\lambda + \rho - \alpha} \frac{q \cdot Q_{co_2}}{\rho - \alpha} \cdot E^*_{ccus,2} + B_{1,imm} \cdot \delta_1 \cdot \left(E^*_{ccus,2}\right)^{\delta_1 - 1} \\ &= \frac{\lambda}{\lambda + \rho - \alpha} \frac{Q}{\rho - \alpha} + B_{4,imm} \cdot \delta_2 \cdot \left(E^*_{ccus,2}\right)^{\delta_2 - 1}.\end{aligned} \tag{A.25}$$

We can summarize the investment decision for Model 4 in Figure A.4. In Stage 1, $F_1(E)$ and $\phi_1(E)$ match at the threshold $E^*_{ccs,1}$, as in Model 2. Figure A.4 (b) shows the solution for Stage 2, where $F_2(E)$ collapses with the value of operating CCUS $V_{ccus}(E)$ at the threshold $E^*_{ccs,2}$.

(*a*) *Stage 1*



(*b*) *Stage 2*

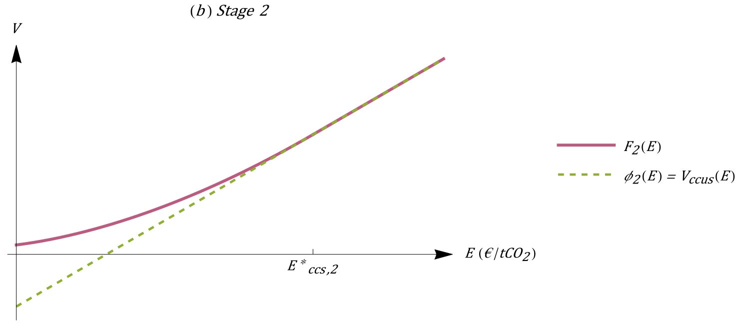


Figure A.4: The firm's investment decision problem in Stage 1 and Stage 2, in Model 4.

A.5 Comparative statics

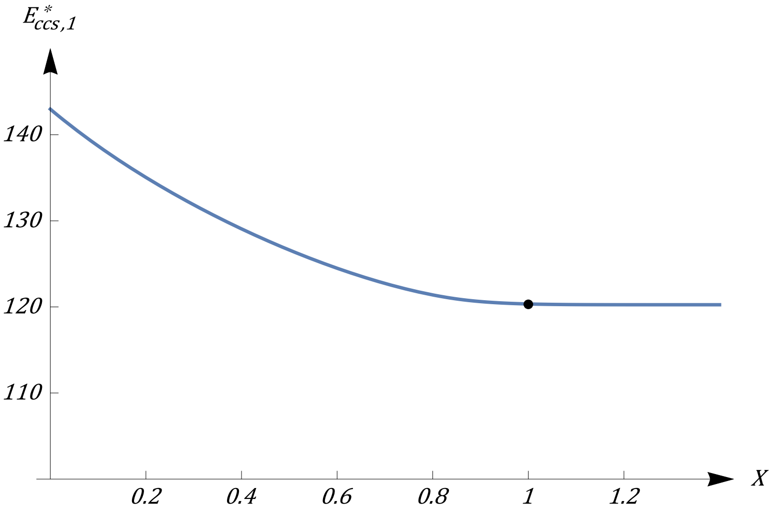


Figure A.5: The influence of X on the investment threshold $E^*_{ccs,1}$.

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