Optimising the design of supply chains for carbon capture, utilisation and sequestration in Europe: a preliminary assessment

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Supplementary Material

1 MATHEMATICAL FORMULATION

This Supplementary Material describes the mathematical formulation adopted to represent the carbon capture utilisation and storage (CCUS) supply chain (SC) which has been discussed in the main text. The objective is to minimise the total cost TC [€] that occurs to install and operate the CCUS network, including the total cost related to capture facilities TCC [€], the total cost of the transport infrastructure TTC [€], the total cost for geologically confining the CO_2 TSC [€], and the $profit$ [€] coming from the utilisation stage:

$$\begin{cases} objective = min(TC) \\ TC = TCC + TTC + TSC - profit \\ s.t. \\ capture\ problem\ model \\ transport\ problem\ model \\ sequestration\ problem\ model \\ utilisation\ problem\ model \end{cases} \tag{S1}$$

In particular, the *capture problem model*, the *transport problem model* and the *sequenstration problem model* will be briefly described in the following (for further information, the full descriptions related to these stages are reported in: d'Amore and Bezzo, 2017; d'Amore et al., 2018), whereas the *utilisation problem model* can be found in the main text.

1.1 The capture problem model

The first SC echelon entails the optimal selection, positioning and sizing of capture technologies, which are described through a set k =$\{post^{comb}_{coal}, post^{comb}_{gas}, oxy^{fuel}_{coal}, pre^{comb}\}$. The total cost for capture TCC of Eq.(S1) is calculated on the basis of the captured flowrate $C_{k,g}$ [t of CO_2] through technology k in region g and the unitary cost for capture UCC_k [€/t of CO_2] for installing and operating a facility k:

$$TCC = \sum_{k,g} (UCC_k \cdot C_{k,g}) \qquad \forall k, g \tag{S2}$$

where the unitary cost UCC_k is evaluated for options k as reported in d'Amore and Bezzo (2017) (Table S1). The captured flowrate $C_{k,g}$ of Eq.(S2) is calculated from the regional processed flowrate $P_{k,g}$ [t of CO_2] through technology k in region g, considering a capture efficiency η_k for technologies k (Table S1):

$$C_{k,g} = \eta_k \cdot P_{k,g} \qquad \forall k, g \tag{S3}$$

Table S1. Capture efficiencies (η_k) and unitary capture cost (UCC_k [€/t of CO_2]) for each technology k. Data retrieved from d'Amore and Bezzo (2017).

	k			
	$post^{comb}_{coal}$	$post^{comb}_{gas}$	oxy^{fuel}_{coal}	pre^{comb}
η_k	0.87	0.88	0.92	0.86
UCC_k	33	54	36	25

The upper bound for the calculation of $P_{k,g}$ of Eq.(S3) is set according to the level of CO_2 emissions from large-stationary sources P^{tot}_g [t of CO_2] in region g, through the following constraints:

$$\sum_k P_{k,g} \leq P^{tot}_g \qquad \forall g \tag{S4}$$

$$P_{k,g} \leq P^{tot}_g \cdot \gamma_{k,g} \qquad \forall k, g \tag{S5}$$

where $\gamma_{k,g}$ describes the feasibility of installing a capture technology k in region g according to the presence of either coal- and/or gas-fed power plants in that specific area, and is retrieved from d'Amore and Bezzo (2017). In particular, P^{tot}_g of Eqs.(S4,S5) is calculated from the CO_2 emissions database provided by JRC (2016) and reported in d'Amore and Bezzo (2017).

1.2 The transport problem model

Once captured, CO_2 must be cost-effectively transported towards either a sequestration basin, or a conversion facility. The set of possible transport means includes l =\{$pipeline^{onshore}$, $pipeline^{offshore}$, $ship$\}. The total cost to install and operate the transport infrastructure TTC of Eq.(S1) is given by the combined contributions of inter-connection costs between regions g and g' accounting for scale effects on size (i.e., TTC^{size} [€]), inter-connection costs between regions g and g' accounting for scale effects of distance (i.e., TTC^{dist} [€]) and of a corrective cost component (i.e., TTC^{intra} [€]) that accounts the intra-connection systems within cells g:

$$TTC = TTC^{size} + TTC^{dist} + TTC^{intra} \tag{S6}$$

Inter-connection costs TTC^{size} of Eq.(S6) are specifically designed for pipeline transport and are evaluated as follows:

$$TTC^{size} = \sum_{p,g,l,g'} (UTC_{p,l} \cdot Q_{p,g,l,g'} \cdot LD_{g,g'} \cdot \tau_g) \tag{S7}$$

where $Q_{p,g,l,g'}$ represents the CO_2 flowrate p (ranging from 1 Mt of CO_2/year to 30 Mt of CO_2/year) that is transported through mode l between regions g and g', τ_g is a tourtuosity factor for region g, $LD_{g,g'}$ [km] is the linear distance between regions g and g', and $UTC_{p,l}$ [€/km/t of CO_2] is the unitary transport cost (Table S2). The parameters $UTC_{p,l}$, τ_g and $LD_{g,g'}$ are taken from d'Amore and Bezzo (2017). Thus, the overall flowrate $Q_{g,l,g'}$ between regions g and g' is given by:

$$Q_{g,l,g'} = \sum_p Q_{p,g,l,g'} \qquad \forall g.l.g' \tag{S8}$$

Conversely, the contribution of TTC^{dist} of Eq.(S6) is only calculated for offshore transport through ships (as suggested in d'Amore and Bezzo, 2017):

$$TTC^{dist} = \sum_{g,l,g'} (f^{ship} \cdot Q_{g,l,g'} \cdot LD_{g,gp}) \qquad \forall l = ship \tag{S9}$$

The parameter f^{ship} [€/km/t] is the curve of unitary costs for ships (Table S2). Finally, intra-connection costs TTC^{intra} of Eq.(S6) take into account the spatial discretization of the proposed formulation through

Table S2. Transport unitary cost $UTC_{p,l}$ [€/km/t of CO_2] according to the discretisation p of transport capacities Q_p [t of CO_2/year]. The constant value for ship transport ($UTC_{p,ship} = 0.03215$ €/km/t of CO_2) is then lowered according to a kilometric slope ($f^{ship} = -0.00001385$ €/km/t of CO_2), the latter representing economies of scale on total transport distance. Data retrieved from d'Amore and Bezzo (2017)

		$UTC_{p,l}$		
p	Q_p [Mt/year]	onshore [€/km/t]	offshore [€/km/t]	ship [€/km/t]
1	1	0.04009	0.07137	0.03215
2	5	0.01476	0.02215	0.03215
3	10	0.00959	0.01338	0.03215
4	15	0.00746	0.00997	0.03215
5	20	0.00624	0.00808	0.03215
6	25	0.00543	0.00687	0.03215
7	30	0.00485	0.00602	0.03215

a grid of squared cells thus, the fact that in general some additional infrastructural expenditures should be taken into account within operating cells g:

$$TTC^{intra} = \sum_{k,g} (\bar{UTC} \cdot C_{k,g} \cdot LD_g) \qquad \text{(S10)}$$

where $\bar{UTC}$ [€/km/t] is an average unitary transport cost evaluated for short distances (i.e., comparable with the size of a cell g), while LD_g [km] is equal to half of the diagonal size of a region g.
The key variable to evaluate the elements of Eqs.(S6-S10) is the CO_2 flowrate $Q_{g,l,g'}$ [t of CO_2] that is transported from region g through mean l to region g'. Having defined both the CO_2 that is captured in region g (i.e., $C_{k,g}$) through Eqs.(S2,S3), and that shipped to region g' (i.e., $Q_{g,l,g'}$) through Eqs.(S7-S10), it is now possible to impose the mass balance in region g:

$$\sum_k C_{k,g} + \sum_{l,g'} Q_{g',l,g} = U_g^{seq} + \sum_{l,g'} Q_{g,l,g'} + \sum_c U_{\psi,g} \qquad \forall g \neq g' \qquad \text{(S11)}$$

where U_g^{seq} [t of CO_2] represents the amount of CO_2 that is geologically sequestered in region g, whereas $U_{\psi,g}$ [t of CO_2] is that CO_2 sent to a conversion and utilisation facility for producing chemical ψ in region g. In particular, this latter $U_{\psi,g}$ of Eq.(S11) is calcolated through the *utilisation problem model*, which is reported in the main text.

1.3 The sequestration problem model

Finally, the CCUS scheme contemplates that CO_2 can be either transported towards a suitable geological basin, or converted into a useful product. On the one side, the utilisation stage is described in the main text, and defines the optimal amount of CO_2 that is sent to industrial use (i.e., $U_{\psi,g}$) to produce either polyether carbonate polyols (PPP) or methanol (MeOH), with the possible chemical outputs described through a set $\psi = \{PPP, MeOH\}$. On the other hand, geological storage involves the optimal positioning and sizing of injection wells. The total sequestration cost TSC of Eq.(S1) is proportional to the number of injection wells N_g that need to be installed in region g:

$$TSC = \sum_g (USC_g \cdot N_g) \qquad \forall g \qquad \text{(S12)}$$

where USC_g [€/well] is the unitary sequestration cost for installing and operating one injection well in region g and its calculation is detailed in d'Amore and Bezzo (2017). On the other hand, N_g of Eq.(S12) depends on the amount of CO_2 that is sequestered in region g according to U_g^{seq} of Eq.(S11) and on the maximum flowrate N^{max} [t of CO_2] that can be processed through a single well (taken from d'Amore and Bezzo, 2017):

$$N_g = N^{max} \cdot U_g^{seq} \qquad \forall g \tag{S13}$$

The upper bound for the calculation of U_g^{seq} of Eq.(S13) is given by the maximum storage availability $U_g^{seq,max}$ [t of CO_2] in region g, which is retrieved from d'Amore and Bezzo on the basis of the results provided by the EUGeoCapacity Project (2018):

$$U_g^{seq} \leq U_g^{seq,max} \qquad \forall g \tag{S14}$$

Table S3. Prices of natural gas (gas p.) and electricity (el. p.), labour cost (lab_c [k€/y]) and corporate tax rate (tax_c) in the analysed countries c (Eurostat, 2017a; 2017b; 2017c).

c	gas p. [€/kWh]	el. p. [€/kWh]	lab_c [k€/y]	tax_c
Belgium	0.0244	0.113	55.691	0.340
Czech Republic	0.0238	0.069	17.480	0.190
Denmark	0.0327	0.082	62.756	0.220
Germany	0.0317	0.152	51.825	0.298
Ireland	0.0332	0.124	49.660	0.125
Greece	0.0283	0.107	28.179	0.290
Spain	0.0310	0.106	36.388	0.250
France	0.0326	0.099	53.384	0.333
Croatia	0.0246	0.087	16.659	0.200
Italy	0.0271	0.148	43.822	0.240
Lithuania	0.0246	0.084	10.263	0.150
Hungary	0.0261	0.074	13.136	0.090
Netherlands	0.0365	0.082	56.107	0.250
Poland	0.0273	0.086	13.227	0.190
Portugal	0.0279	0.114	22.321	0.210
Romania	0.0255	0.079	7.648	0.160
Slovakia	0.0282	0.112	15.205	0.210
Finland	0.0441	0.067	50.376	0.200
United Kingdom	0.0248	0.127	47.068	0.190
Macedonia	0.0300	0.056	6.626	0.100
Albania	0.0578	0.084	4.626	0.150
Serbia	0.0310	0.064	8.404	0.150
Turkey	0.0187	0.063	13.899	0.200
Bosnia	0.0343	0.059	9.702	0.100
Moldova	0.0263	0.083	3.600	0.120
Ukraine	0.0262	0.039	3.352	0.190

2 PARAMETERS AND TABLES

This section provides additional information, parameters and tables employed to set up the CCUS SC described in the main text. In particular, Table S3 displays the price of electricity [€/kWh], labour cost [k€/y], corporate tax rate [%], and the price of natural gas [€/kWh] in the analysed European countries c. Table S4 shows the cost of raw materials $raw_{\psi,g}$ [€/t of chemical] for producing chemical ψ in region g, while the corresponding cost of utilities $util_{\psi,g}$ is reported in Table S5. These parameters are employed in the main text for the calculation of costs of chemicals ψ, and are retrieved from Eurostat statistics (Eurostat, 2017a; 2017b; 2017c). On the other hand, regional carbon intensities for electricity generation CI_g [t of indirect CO_2/GJ] are described in Table S6 for each region g (ElectricityMap, 2019; EEA, 2019; IEA, 2019).

Table S4. Cost of raw materials $raw_{\psi,g}$ [€/t of chemical] for producing chemical ψ in region g (Eurostat, 2017a; 2017b; 2017c), with null values for offshore cells g ={125, ..., 134}.

	ψ			ψ			ψ	
g	PPP [€/t]	MeOH [€/t]	g	PPP [€/t]	MeOH [€/t]	g	PPP [€/t]	MeOH [€/t]
1	1386.6	326.9	43	1386.6	195.1	85	1386.6	210.1
2	1386.6	326.9	44	1386.6	195.1	86	1386.6	210.1
3	1386.6	326.9	45	1386.6	169.6	87	1386.6	210.1
4	1386.6	326.9	46	1386.6	169.6	88	1386.6	210.1
5	1386.6	326.9	47	1386.6	222.9	89	1386.6	210.1
6	1386.6	326.9	48	1386.6	222.9	90	1386.6	176
7	1386.6	326.9	49	1386.6	222.9	91	1386.6	176
8	1386.6	381.1	50	1386.6	219.4	92	1386.6	176
9	1386.6	326.9	51	1386.6	219.4	93	1386.6	176
10	1386.6	326.9	52	1386.6	166.7	94	1386.6	290.1
11	1386.6	326.9	53	1386.6	166.7	95	1386.6	198.6
12	1386.6	170.2	54	1386.6	170.2	96	1386.6	185.8
13	1386.6	170.2	55	1386.6	170.2	97	1386.6	185.8
14	1386.6	381.1	56	1386.6	169.6	98	1386.6	127.9
15	1386.6	381.1	57	1386.6	169.6	99	1386.6	199.1
16	1386.6	196.8	58	1386.6	169.6	100	1386.6	210.1
17	1386.6	196.8	59	1386.6	222.9	101	1386.6	210.1
18	1386.6	196.8	60	1386.6	222.9	102	1386.6	210.1
19	1386.6	213.1	61	1386.6	176	103	1386.6	210.1
20	1386.6	213.1	62	1386.6	176	104	1386.6	210.1
21	1386.6	170.2	63	1386.6	176	105	1386.6	176
22	1386.6	170.2	64	1386.6	178.3	106	1386.6	176
23	1386.6	256.5	65	1386.6	192.2	107	1386.6	176
24	1386.6	219.4	66	1386.6	184.1	108	1386.6	185.8
25	1386.6	219.4	67	1386.6	184.1	109	1386.6	185.8
26	1386.6	219.4	68	1386.6	184.1	110	1386.6	127.9
27	1386.6	219.4	69	1386.6	165	111	1386.6	127.9
28	1386.6	195.1	70	1386.6	199.1	112	1386.6	210.1
29	1386.6	195.1	71	1386.6	195.1	113	-	-
30	1386.6	195.1	72	1386.6	195.1	114	-	-
31	1386.6	195.1	73	1386.6	195.1	115	-	-
32	1386.6	195.1	74	1386.6	222.9	116	-	-
33	1386.6	170.2	75	1386.6	176	117	-	-
34	1386.6	170.2	76	1386.6	176	118	-	-
35	1386.6	170.2	77	1386.6	176	119	1386.6	176
36	1386.6	169.6	78	1386.6	233.3	120	1386.6	176
37	1386.6	219.4	79	1386.6	233.3	121	1386.6	185.8
38	1386.6	219.4	80	1386.6	197.4	122	1386.6	185.8
39	1386.6	219.4	81	1386.6	184.1	123	1386.6	185.8
40	1386.6	219.4	82	1386.6	184.1	124	1386.6	127.9
41	1386.6	195.1	83	1386.6	184.1			
42	1386.6	195.1	84	1386.6	199.1			

Table S5. Cost of utilities $util_{\psi,g}$ [€/t of chemical] for producing chemical ψ in region g (Eurostat, 2017a; 2017b; 2017c), with null values for offshore cells $g = \{125, ..., 134\}$.

g	ψ PPP [€/t]	ψ MeOH [€/t]	g	ψ PPP [€/t]	ψ MeOH [€/t]	g	ψ PPP [€/t]	ψ MeOH [€/t]
1	3.24	145.4	43	3.08	130.1	85	3.01	128.3
2	3.24	145.4	44	3.08	130.1	86	3.01	128.3
3	3.24	145.4	45	1.92	82.1	87	3.01	128.3
4	3.24	145.4	46	1.92	82.1	88	3.01	128.3
5	3.24	145.4	47	2.92	125.4	89	3.01	128.3
6	3.24	145.4	48	2.92	125.4	90	3.26	135.8
7	3.24	145.4	49	2.92	125.4	91	3.26	135.8
8	5.43	236.4	50	3.77	159.3	92	3.26	135.8
9	3.24	145.4	51	3.77	159.3	93	3.26	135.8
10	3.24	145.4	52	2.26	95.4	94	10.03	393.9
11	3.24	145.4	53	2.26	95.4	95	2.27	98.1
12	3.01	125.5	54	3.03	128.1	96	2.79	117.7
13	3.01	125.5	55	3.03	128.1	97	2.79	117.7
14	5.43	236.4	56	1.92	82.1	98	1.93	79.6
15	5.43	236.4	57	1.92	82.1	99	3.08	130.1
16	2.65	113.0	58	1.92	82.1	100	3.01	128.3
17	2.65	113.0	59	2.92	125.4	101	3.01	128.3
18	2.65	113.0	60	2.92	125.4	102	3.01	128.3
19	3.14	133.8	61	3.26	135.8	103	3.01	128.3
20	3.14	133.8	62	3.26	135.8	104	3.01	128.3
21	3.01	125.5	63	3.26	135.8	105	3.26	135.8
22	3.01	125.5	64	2.50	105.6	106	3.26	135.8
23	2.99	130.5	65	2.51	107.2	107	3.26	135.8
24	3.77	159.3	66	2.46	104.4	108	2.79	117.7
25	3.77	159.3	67	2.46	104.4	109	2.79	117.7
26	3.77	159.3	68	2.46	104.4	110	1.93	79.6
27	3.77	159.3	69	2.33	98.0	111	1.93	79.6
28	3.08	130.1	70	3.08	130.1	112	3.01	128.3
29	3.08	130.1	71	3.01	128.3	113	-	-
30	3.08	130.1	72	3.01	128.3	114	-	-
31	3.08	130.1	73	3.01	128.3	115	-	-
32	3.08	130.1	74	2.92	125.4	116	-	-
33	3.01	125.5	75	3.26	135.8	117	-	-
34	3.01	125.5	76	3.26	135.8	118	-	-
35	3.01	125.5	77	3.26	135.8	119	3.26	135.8
36	2.81	117.4	78	2.52	110.4	120	3.26	135.8
37	3.77	159.3	79	2.52	110.4	121	2.79	117.7
38	3.77	159.3	80	2.34	100.6	122	2.79	117.7
39	3.77	159.3	81	2.46	104.4	123	2.79	117.7
40	3.77	159.3	82	2.46	104.4	124	1.93	79.6
41	3.08	130.1	83	2.46	104.4			
42	3.08	130.1	84	2.58	107.9			

Table S6. Electricity generation carbon intensity CI_g [t of indirect CO_2/GJ] in regions g, with null values for offshore cells $g = \{125, ..., 134\}$ (ElectricityMap, 2019; EEA, 2019; IEA, 2019). Regions g with the same value pertain to the same country.

g	CI_g [t/GJ]	g	CI_g [t/GJ]	g	CI_g [t/GJ]	g	CI_g [t/GJ]
1	0.03133	32	0.21481	63	0.07058	94	0.00250
2	0.03133	33	0.07808	64	0.05833	95	0.40278
3	0.03133	34	0.07808	65	0.07233	96	0.17306
4	0.03133	35	0.07808	66	0.08500	97	0.17306
5	0.03133	36	0.04711	67	0.08500	98	0.13306
6	0.03133	37	0.12244	68	0.08500	99	0.09019
7	0.03133	38	0.12244	69	0.17694	100	0.07372
8	0.03225	39	0.12244	70	0.09019	101	0.07372
9	0.03133	40	0.12244	71	0.07372	102	0.07372
10	0.03133	41	0.21481	72	0.07372	103	0.07372
11	0.03133	42	0.21481	73	0.07372	104	0.07372
12	0.07808	43	0.21481	74	0.01625	105	0.07117
13	0.07808	44	0.21481	75	0.07117	106	0.07117
14	0.03225	45	0.07583	76	0.07117	107	0.07117
15	0.03225	46	0.07583	77	0.07117	108	0.17306
16	0.00500	47	0.01625	78	0.13061	109	0.17306
17	0.00500	48	0.01625	79	0.13061	110	0.13306
18	0.00500	49	0.01625	80	0.10056	111	0.13306
19	0.11803	50	0.12244	81	0.08500	112	0.07372
20	0.11803	51	0.12244	82	0.08500	113	0.25586
21	0.07808	52	0.02364	83	0.08500	114	0.25586
22	0.07808	53	0.14242	84	0.09019	115	0.25586
23	0.14033	54	0.03675	85	0.07372	116	0.25586
24	0.12244	55	0.03675	86	0.07372	117	0.18056
25	0.12244	56	0.07583	87	0.07372	118	0.18056
26	0.12244	57	0.07583	88	0.07372	119	0.07117
27	0.12244	58	0.07583	89	0.07372	120	0.07117
28	0.21481	59	0.01625	90	0.07117	121	0.17306
29	0.21481	60	0.00389	91	0.07117	122	0.17306
30	0.21481	61	0.07117	92	0.07117	123	0.17306
31	0.21481	62	0.07117	93	0.07117	124	0.13306

NOMENCLATURE

Acronyms

CCUS	Carbon dioxide capture, utilisation, and storage
MeOH	Methanol
PPP	Polyether carbonate polyols
SC	Supply chain

Sets

g	Region, g ={1, 2, ..., 133, 134}
k	Capture technology, $k = \{post^{comb}_{coal}, post^{comb}_{gas}, oxy^{fuel}_{coal}, pre^{comb}\}$
l	Transport mode, $l = \{pipeline^{onshore}, pipeline^{offshore}, ship\}$
p	Flowrate, p ={1, 2, ..., 6, 7}
ψ	Chemical output, $\psi = \{PPP, MeOH\}$

Parameters

CI_g	Electricity carbon intensity in region g [t/GJ]
$\gamma_{k,g}$	Feasibility of installing technology k in region g
$lab_{\psi,g}$	Labour cost for producing chemical ψ in region g [€/t]
eta_k	Capture efficiency of technology k
f^{ship}	Cost curve for ships [€/km/t]
LD_g	Half of diagonal size of cell g [km]
$LD_{g,g'}$	Linear distance between region g and g' [km]
N^{max}	Maximum flowrate that can be processed through a single well [t/well]
P^{tot}_g	Total emissions in region g [t]
Q_p	Discretized transported flowrate [t]
$raw_{\psi,g}$	Unitary cost of raw materials for producing chemical ψ in region g [€/t]
tax_g	Taxation in region g
τ_g	Tourtuosity factor in region g
UCC_k	Unitary capture cost through technology k [€/t]
$U\bar{T}C$	Average unitary transport cost [€/km/t]
USC_g	Unitary sequestration cost [€/well]
$U^{seq,max}_g$	Maximum storage availability in region g [t]
$UTC_{p,l}$	Unitary transport cost for flowrate p through mean l [€/km/t]
$util_{\psi,g}$	Unitary cost of utilities for producing chemical ψ in region g [€/t]

Variables

$C_{k,g}$	Captured flowrate through technology k in region g [t]
N_g	Number of installed injection wells in region g [wells]
$P_{k,g}$	Processed flowrate through technology k in region g [t]
$profit$	Total profit from the sale of chemicals [€]
$Q_{g,l,g'}$	Total transported flowrate from g through l to g' [t]
$Q_{p,g,l,g'}$	Transported flowrate p from g through l to g' [t]
TC	Total cost [€]
TCC	Total capture cost [€]
TSC	Total sequestration cost [€]
TTC	Total transport cost [€]
TTC^{size}	Inter-connection cost with scale effects on size [€]
TTC^{dist}	Inter-connection cost with scale effects on distance [€]
TTC^{intra}	Intra-connection cost [€]
U^{seq}_g	Sequestered amount in region g [t]
$U_{\psi,g}$	Flowrate sent to a conversion facility for producing ψ in region g [t]

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