Supplementary Information (SI) for Sustainable Energy & Fuels.

Appendix I / Online Support Information (SI) file (if needed)

In Appendix I, Table A1 summarizes the eight GEC and their respective chemical properties. These values form the basis for the both p- & s-ETC frameworks.

Table A1. The chemical properties the selected GEC (31).

GEC	**Abbr.**	**Chemical Formula**	**Trans/ phase** p- or s-	**Densities** mass Kg/m^3	m-Energy MJ/kg	V-Energy MJ/l	Hydro. wt.%	**Liquid Temp.** °C at 1 atm
[1]**Hydrogen***	**H_2**	H_2	p- s-	g: 5.3 l: 71.0	120.0	g: 0.6 l: 8.5	100.0	-259 ↔ -253
[1]**Methane**	**CH_4**	CH_4	p- s-	g: 82.6 l: 424.0	55.0	g: 4.5 l: 23.2	25.0	-183 ↔ -161
[2]**Ammonia***	**NH_3**	NH_3	p-; s-	g: N.R. l: 629.0	18.6	g: N.R. l: 11.7	17.8	-78 ↔ -33
[2]**Methanol**	**MeOH**	CH_4O	p-; s-	g: N.R. l: 792.0	19.9	g: N.R. l: 15.8	12.1	-98 ↔ 65
[2]**Ethanol**	**EtOH**	C_2H_6O	p-; s-	g: N.R. l: 789.0	26.8	g: N.R. l: 21.1	13.0	-98 ↔ 65
[3]**Toluene-methylcyclohexane***	**TMCH**	a: C_7H_8 b: C_7H_{14}	p-; s-	g: N.R. l: 770.0	7.4	g: N.R. l: 5.7	15.5	-126 ↔ 101
[3]**Synthetic Paraffinic Kerosene**	**SPK**	C_8-C_{16} Chains	p-; s-	g: N.R. l: 757.0	44.1	g: N.R. l: 33.4	6.1	-47 ↔ 176
[3]**Formic Acid**	**FA**	CH_2O_2	p-; s-	g: N.R. l: 1220.0	5.5	g: N.R. l: 6.7	4.4	8 ↔ 101

N.B. *** = framework backbone GEC**; **1 = G1; 2 = G2; 3 = G3; Trans/phase = transport medium & phase designation;** abbr. = abbreviations; Hydro. = Hydrogen; a = toluene; b = methylcyclohexane; m- = mass; V- = volumetric; g = gaseous phase; l = liquid phase; N.R. = not relevant.

Appendix II

In Appendix II, we present the main equations used in our study. Equation 1.1 represents the ETC formula discussed in Section 2.2, which is essential for deriving the desired unit of output [M€/PJ]. Equation 1.2 shows the calculation for total annual costs. Equation 3 depicts the formula for annuitization, necessary to annuitize all non-yearly costs.

Main Equations

$$ETC\ [M€/PJ] = \frac{TAC\ [€/yr]}{Q_{true}\ [kt/\mathrm{yr}] \times EC_{GEC}\ [MJ/kg]} \qquad (Eq. 1.1)$$

$$TAC\ [M€/yr] = (AF\ [yr^{-1}] \times total\ CAPEX\ [M€]) + total\ OPEX\ [M€/yr] \qquad (Eq. 1.2)$$

$$Annuity\ factor\ (AF) = \frac{interest\ rate\ [\%]}{1-(1+interest\ rate\ [\%])^{(-lifetime\ [yr])}} \qquad (Eq. 3)$$

Table A2. Pipeline parameters (ETSAP, 2011).

Abbreviation/Symbol	Unit	Value	Definition
ETC	**M€/PJ**	-	Energy Transportation Cost
TAC	**M€/yr**	-	Total Annual Cost
Q_{true}	**Kt/yr**	-	True GEC Throughput
EC_{GEC}	**MJ/kg**	-	GEC Energy Density

Appendix III

Here, we delineate the step-by-step equation pathway for calculating the pipeline framework, essential for solving Equation 1.1. We begin by computing the pipeline diameter (Eq. 4), leveraging the equation detailed by Baufumé et al., (2013) to derive the CAPEX per kilometer. The total CAPEX is then determined, factoring in the TD and annuitization using Eq. 3 from Appendix II, which considers pipeline lifetime and discount rates. Furthermore, Equations 6.1 and 6.2 specify the actual GEC throughput values for gas and oil pipelines, respectively. These equations account for pipeline utilization rates and loss factors, where each kilometer and CP-station contributes to overall efficiency losses. Lastly, equations 7 and 8 provide the methodology for calculating the total number of CP-stations required for a given TD, encompassing all relevant costs.

Pipeline Equations for any chosen TD

$$D\ [m] = \sqrt{\frac{4 \times Q_{design}\ [kg/s]}{\rho\ [kg/m^3] \times v\ [m/s] \times \pi}} \qquad D \geq 0.1 \qquad (Eq. 4)$$

$$CAPEX\ [€/km] = 4\ 000\ 000 D^2 + 598\ 600 D + 329\ 000 \qquad (Eq. 5)$$

$$(Q_{true})_o [kt/\mathrm{yr}] = Q_{design}[kt/yr] \times UR\ [\%/100](1 - LF_o[\%/100km\text{-}CP_{station}] \times TD\ [km]) \qquad (Eq. 6.1)$$

$$(Q_{true})_g [kt/yr] = Q_{design}[kt/\mathrm{yr}] \times UR[\%/100](1 - LF_g[\%/100km\text{-}CP_{station}] \times TD[km]) \qquad (Eq. 6.2)$$

$$n\ CP_{station}^{parallel}\ [int] = \frac{Q_{daily}\ [t/day]}{Q_{station}^{Max}\ [t/day]} \qquad (Eq. 7)$$

$$n\ CP_{station}^{total}\ [int] = n\ CP_{station}^{parallel}\ [int] \times \frac{TD\ [km]}{CP_{distance}^{average}\ [km]} \qquad (Eq. 8)$$

Table A3. Pipeline parameters (ETSAP, 2011).

Abbreviation/Symbol	Unit	Value	Definition
D	**m**	-	Diameter
ρ	**Kg/m^{-3}**	-	Mass Density
v	**m/s**	-	Flow Speed
CAPEX	**€/km**	-	Pipeline Construction Cost per Km
Q_{design}	**Kt/yr**	-	Design GEC Throughput
UR	**%/100**	-	Utilisation Rate
TD	**km**	-	Transportation Distance
LF_o	**%/100km-CP$_{station}$**	G2: 3.33E-5 G3: 1.00E-5	Oil Loss Factor[1]
LF_g	**%/100km-CP$_{station}$**	G1: 1.50E-4	Gas Loss Factor[1]
$n\ CP_{station}^{parallel}$	**integer**	-	Number of parallel CP-stations
Q_{daily}	**t/day**	-	Daily GEC throughput
$Q_{station}^{Max}$	**t/day**	-	Max CP-station throughput
$n\ CP_{station}^{total}$	**integer**	-	Total number of CP-stations for a given TD
$CP_{distance}^{average}$	**km**	-	Average distance between CP-stations

N.B. [1] = The loss factors are based on specific leakage and GEC usage values which can be found in SIII.

Appendix IV

In this section, we present a detailed step-by-step guide outlining the calculation process for shipping, which is essential for computing the ETC values for selected GECs (Eq. 1.1, Appendix II). The sequence begins with Equation 9, determining the total roundtrip time of a ship, a crucial parameter for calculating the true GEC throughput per chosen TD (Eq. 10). Next, Equation 11 converts the GEC throughput per trip to a yearly rate, aligning with the timeframe of our study. Equations 12.1 and 12.2 constitute the core calculations to obtain the true GEC throughput required for Equation 1.1 (Appendix II). While Equation 11.1 is straightforward, Equation 11.2 involves additional steps to reach the desired value. Subsequent formulas (Eq. 13.1, 13.2, and 13.3) account for various losses such as boil-off and flash rates, with Equation 13.3 incorporating storage parameters to determine minimal GEC storage requirements before local distribution. Cost considerations are addressed through Equations 14.1, 14.2, and 14.3, where integer outputs reflect the operational constraints such as the absence of half ships and terminals. Importantly, the number of ships influences the Q_{true} in Equation 9, which is pivotal for subsequent calculations where the ship's GEC storage capacity determines the rate-limiting step.

On the following page, Table A4 provides further clarification on abbreviations and units used, while detailed cost data can be found in SIV

Shipping Equations for any chosen TD

$$TRT\ [day] = \frac{TD[km]}{12v[m/s]} + t_{load}[day] + t_{unload}[day] \qquad (Eq. 9)$$

$$Q_{true}\ [t] = \frac{Q_{prod.}\ [t\ /\ day]\ \times\ TRT\ [day]}{n\ ship} \qquad (Eq. 10)$$

$$ATF\ [yr^{-1}] = \frac{365\ [day] \times UR\ [\%/100]}{TRT\ [day]} \qquad (Eq. 11)$$

$$(Q_{annual})_o\ [t/yr] = Q_{true}\ [t] \times ATF\ [yr^{-1}] \qquad (Eq. 12.1)$$

$$(Q_{annual})_g\ [t/yr] = \Big(\Big(\big(Q_{true}\ [t] - L_{exp}\ [t]\big) - L_{ship}\ [t]\Big) - L_{imp}\ [t]\Big) \times ATF\ [yr^{-1}] \qquad (Eq. 12.2)$$

$$L_{exp}\ [t] = Q_{true}\ [t] \times L_{boil}^{export}\ [\%/100day] \times (TRT\ [day]) + Q_{true}\ [t] \times L_{flash}^{export}\ [\%/100Q_{true}] \qquad (Eq. 13.1)$$

$$L_{ship}\ [t] = Q_{true}^{*}\ [t] \times L_{boil}^{ship}\ [\%/100day] \times \big(t_{transport}\ [day]\big) + Q_{true}^{*}\ [t] \times L_{flash}^{ship}\ [\%/100Q_{true}^{*}] \qquad (Eq. 13.2)$$

$$L_{imp}\ [t] = Q_{true}^{**}\ [t] \times L_{boil}^{import}\ [\%/100day] \times \big(t_{unload}\ [day] + t_{storage}\ [day]\big) \qquad (Eq. 13.3)$$

$$n\ export\ [int] = \frac{Q_{true}\ [t]}{Cap_{terminal}^{export}\ [t]} \quad ; if\ Q_{true} > Cap_{terminal}^{export} \to n+1 \qquad (Eq. 14.1)$$

$$n\ ship\ [int] = \frac{Q_{true}^{*}\ [t]}{Cap_{storage}^{ship}\ [t]} \quad ; if\ Q_{true}^{*} > Cap_{storage}^{ship} \to n+1 \qquad (Eq. 14.2)$$

$$n\ import\ [int] = \frac{Q_{true}^{**}\ [t] + (Q_{true}^{**}\ [t] \times \frac{20\ [day]}{TRT\ [day] \times n\ ships}}{Cap_{terminal}^{import}\ [t]} \quad ; if\ Q_{true}^{**} > Cap_{terminal}^{import} \to n+1 \qquad (Eq. 14.3)$$

Table A4. Shipping parameters (SIV).

Abbreviation/Symbol	Unit	Description
TRT	**day**	Total Roundtrip Time
TD	**km**	Transport Distance
v	**Km/h**	Ship Speed
t_{load}	**day**	Loading time
t_{unload}	**day**	Unloading time
Q_{true}	**t**	True GEC throughput
$Q_{prod.}$	**t/day**	GEC production
n ship	**integer**	Number of ships
ATF	**yr^{-1}**	Annual Time Factor
UR	**%/100**	Utilization Rate
$(Q_{annual})_o$	**t/yr**	Oil: Total GEC throughput
$(Q_{annual})_g$	**t/yr**	Gas: Total GEC throughput
L_{exp}	**t**	Export Loss
L_{ship}	**t**	Shipping Loss
L_{imp}	**t**	Import Loss
L_{boil}^{export}	**%/100day**	Export Boil-off Loss
L_{flash}^{export}	**%/100Q_{true}**	Export Flash-rate Loss
Q_{true}^{*}	**t**	True GEC throughput - L_{exp}
L_{boil}^{ship}	**%/100day**	Shipping Boil-off Loss
$t_{transport}$	**day**	GEC transport time
L_{flash}^{ship}	**%/100Q^*_{true}**	Shipping Flash-rate Loss
Q_{true}^{**}	**t**	True GEC throughput – (L_{exp}+L_{ship})
L_{boil}^{import}	**%/100day**	Import Boil-off Loss
$t_{storgae}$	**day**	Minimal Storage Time
n export	**integer**	Number of export terminals
$Cap_{terminal}^{export}$	**t**	GEC Capacity Export Terminal
$Cap_{storage}^{ship}$	**t**	GEC Storage Capacity Ship
n import	**integer**	Number of import terminals
$Cap_{terminal}^{import}$	**t**	GEC Capacity Import Terminal

N.B. …

Appendix V

In this section, we present the equations essential for computing the devised scoring methods. Equation 15 computes the ETC-score by normalizing the ETC relative to the most expensive GEC. This involves dividing all other ETC values by the highest one, resulting in scores ranging from 0 to 1, where 0 indicates the best performance and 1 indicates the worst.

Similarly, Equations 16 and 17 follow the same methodology, producing three distinct scores also ranging from 0 to 1, where lower values indicate better performance

Scoring Equations

$$H_{score} = \frac{H_{total}^{points}}{H_{GEC}^{points}} \quad ; [0 \leftrightarrow 1] \qquad (Eq. 15)$$

$$R_{score} = \frac{R_{total}^{points}}{R_{GEC}^{points}} \quad ; [0 \leftrightarrow 1] \qquad (Eq. 16)$$

$$ETC_{score} = \frac{ETC_{GEC}^{highest}}{ETC_{GEC}} \quad ; [0 \leftrightarrow 1] \qquad (Eq. 17)$$

Table A5. Score parameters (SII).

Parameter	Unit	Abbreviation/Symbol
Hazard score	-	H_{score}
Rigidity score	-	R_{score}
Energy Transportation Cost score	-	ETC_{score}

Supplementary Information

https://www.dropbox.com/scl/fo/xi37gwzwwisim7xnwlhry/AK1zO2eMNpkSgdgpX4AUDSY?rlkey=vqkpiwfxqhbwixz0ja2vb0dgx&dl=0