Supporting Information

Economic and Environmental Assessment of Asphaltene-derived Carbon Fiber Production

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Table S1 Specific heat values at constant pressure for materials/chemicals

Materials/Chemicals	Specific heat at constant pressure, C_p (kJ/kg-K)	References
Asphaltene	2.20	[1]
Carbon Fiber	1.60	[2]
Toluene (liquid)	1.70	[3]
Toluene (gas)	1.13	[3]
Air	1.00	[4]
Nitrogen	1.04	[5]

Energy calculation for asphaltene-derived carbon fiber (A-CF) production

For various process steps of producing A-CF, the heat is calculated by using the following equation with the help of Table S1-

$$Q = m * c_p * \Delta T \qquad (1)$$

Here,

$Q = heat$

$m = mass$

$c_p = specific\ heat\ at\ constant\ pressure$

$\Delta T = temperaute\ difference$

Calculations for the heat requirement for the various process steps to produce 1 kg of A-CF are shown below:

Heat required for heat treatment:

The heat treatment of treated asphaltene takes place at $280°C$. Using equation 1, the energy required for heat treatment is calculated as follows -

$$Q_1 = m * c_p * \Delta T = 1.77\ kg * 2.2\ \frac{kJ}{kg.K} * (553.15\ K - 303.15\ K) = 973.50\ kJ$$

The heat treatment lasts three hours. Heat loss for one hour is 10%. So, for 3 hours, 30% of heat will be lost. Total heat required for heat treatment -

$$Q_{ht} = Q_1 * 1.30 = 973.50\ kJ * 1.30 = \mathbf{1265.55\ kJ}$$

<u>Heat required for spinning:</u>

Spinning is done at 260°C on heat-treated asphaltene. The heat required for spinning -

$$Q_{sp} = m * c_p * \Delta T = 1.77\ kg * 2.2\ \frac{kJ}{kg.K} * (533.15\ K - 303.15\ K) = \mathbf{895.62\ kJ}$$

Due to the instantaneous spinning, heat loss during this process is not considered.

<u>Heat required for stabilization:</u>

In stabilization, the green fiber is heated in two steps. The fibers are first heated to 260°C for two hours, then to 350°C for one hour. The heat required for fiber stabilization including heat loss is as follows:

$$Q_{stab-f} = m * c_p * \Delta T$$

$$= 1.66\ kg * 1.6\ \frac{kJ}{kg.K}$$

$$* \{(533.15\ K - 303.15\ K) * 1.2 + (623.15 - 533.15) * 1.1\} = 996\ kJ$$

A constant flow of air is circulated into the furnace during stabilization, taking out heat in the process. Heat carrying out by air from 30°C to 260°C –

$$Q_{air-260^{\circ}C} = mass\ flow\ of\ air * total\ duration\ * c_p * \Delta T$$

$$= 1.78x10^{-3}\frac{kg}{s} * 7200\ s * 1\ \frac{kJ}{kg.K} * (533.15\ K - 303.15\ K) = \ 2947.68\ kJ$$

Heat carrying out by air from 260°C to 350°C –

$$Q_{air-350^{\circ}C} = mass\ flow\ of\ air * total\ duration\ * c_p * \Delta T$$

$$= 1.78x10^{-3}\frac{kg}{s} * 3600\ s * 1\ \frac{kJ}{kg.K} * (623.15 - 533.15) = \ 576.72\ kJ$$

Heat carrying out by air including heat loss -

$$Q_{air} = Q_{air-260^{\circ}C} * 1.20 + Q_{air-350^{\circ}C} * 1.10 = 2947.68\ kJ * 1.2 + 576.72\ kJ * 1.1$$
$$= \mathbf{4171.60\ kJ}$$

Heat required for carbonization:

The stabilized fiber is heated in two steps during carbonization. First, it is heated from 30°C to 500°C for half an hour, followed by 1500°C for one hour. The required amount of heat for stabilized fiber is as follows:

$$Q_{car-f} = m * c_p * \Delta T$$
$$= 1.35\ kg * 1.6\ \frac{kJ}{kg.K}$$
$$* \{(773.15\ K - 303.15\ K) * 1.05 + (1773.15 - 773.15) * 1.10\} = 3441.96\ kJ$$

During carbonization, the nitrogen gas is also flowing into the furnace. Heat carrying out by nitrogen from 30°C to 500°C –

$$Q_{N2-500^{\circ}C} = mass\ flow\ of\ nitrogen * total\ duration\ * c_p * \Delta T$$
$$= 1.83x10^{-4} \frac{kg}{s} * 1800\ s * 1.04\ \frac{kJ}{kg.K} * (773.15\ K - 303.15\ K) = 161.01 kJ$$

Heat carrying out by nitrogen from 500°C to 1500°C –

$$Q_{N2-1500^{\circ}C} = mass\ flow\ of\ nitrogen * total\ duration\ * c_p * \Delta T$$
$$= 1.83x10^{-4} \frac{kg}{s} * 3600\ s * 1.04\ \frac{kJ}{kg.K} * (1773.15\ K - 773.15\ K)$$
$$= 685.15\ kJ$$

Total heat carrying out by nitrogen including heat loss -

$$Q_{N2} = Heat_{N2-500^{\circ}C} * 1.05 + Heat_{N2-1500^{\circ}C} * 1.10 = 161.01\ kJ * 1.05 + 685.15\ kJ * 1.1$$
$$= 922.73\ kJ$$

Total energy requirement for the CF production process (without solvent recovery) –

$$Q_{total} = Q_{ht} + Q_{sp} + Q_{stab-f} + Q_{air} + Q_{car-f} + Q_{N2}$$

$$= 1265.55\ kJ + 895.62\ kJ + 996\ kJ + 4171.60\ kJ + 3441.96\ kJ + 922.73\ kJ = 11693.46\ kJ$$

$$\cong \mathbf{3.25}\,\frac{\textbf{kWh}}{\textbf{kg CF}}$$

<u>Calculation of solvent (toluene) recovery energy</u>

Toluene is used as a solvent for A-CF production, in which the raw asphaltene is dissolved in toluene to eliminate any residual solids. Given the substantial quantity of toluene required for the asphaltene pretreatment, the recovery of toluene is essential to reduce production costs and ensure environmental protection. Specifically, to dissolve 1 kg of raw asphaltene, 12.93 kg of toluene is required. With a mass yield of 49.69%, 26.02 kg of toluene is required per kilogram of A-CF. The majority of the toluene can be reclaimed by boiling and condensation, with an estimated recovery rate of approximately 98%.

$$Amount\ of\ toluene\ to\ recover = Toluene\ required\ per\ kg\ of\ carbon\ fiber\ * recovery\ rate$$

$$Amount\ of\ toluene\ to\ recover = 26.02\ kg * 0.98 = 25.50\ kg$$

The recovery process for toluene involves heating it to a temperature approximately 10°C above its boiling point and subsequently condensing it at room temperature.

The total amount of heat required to recover toluene per kg of A-CF is calculated as follows:

$$Q_{tol} = m_l * c_{p1} * (t_b - t_r) + m_l * l_f + m_l * c_{p2} * \left(t_f - t_b\right)$$

$$Q_{tol} = 25.50\ kg * 1.7\ \frac{kJ}{kg.K} * (383.75\ K - 303.15\ K) + 25.50\ kg * 413\ \frac{kJ}{kg} + 25.50 * 1.13\ \frac{kJ}{kg.K} * (393.75\ K - 383.75\ K) = 14287.65\ \frac{kJ}{kg} \cong \mathbf{3.97}\,\frac{\textbf{kWh}}{\textbf{kg}}$$

Here,

$m_l = mass\ of\ toluene\ to\ recover,$

$c_{p1} = specific\ heat\ of\ liquid\ toluene\ at\ const.pressure$

$c_{p2} = specific\ heat\ of\ toluene\ gas\ at\ const.pressure$

$l_f = Toluene\ heat\ (enthalpy) of\ evaporation$

$t_b = boiling\ point\ temperature\ of\ toluene$

$t_r = room\ temperature$

$t_f = final\ temperature$

As the boiling point temperature is approximately 80°C higher than the room temperature, condensation of toluene vapor doesn't need any external energy.

<u>Calculation for the fixed cost of A-CF production:</u>

Table S2 Capital cost for equipment of an A-CF plant capable of producing 2000 tonnes/year[6,7]

Equipment	**Million USD (April 2022)**
Pre-treatment equipment	2.79
Melt-spinning machine	3.49
Stabilization oven	8.38
Carbonization oven	9.77
Post-processing equipment	5.59
Installation, commissioning	16.90
Drivers, rollers, ancillary, etc.	8.66
Overhead cost	6.18
Total cost	61.76

Capital cost for equipment is calculated as annuity over the expected lifetime by using the following equation:

$$Annual\ cost = Capital\ investment \times \frac{r \times (1+r)^n}{(1+r)^n - 1}$$

$$= \$61.76 \times 10^6\ for\ 2000 \frac{tonnes}{year} \times \frac{0.1 \times (1+0.1)^{25}}{(1+0.1)^{25} - 1}$$

$$= \$6.80 \times 10^6\ for\ 2000 \frac{tonnes}{year}$$

$$= \$3.40\ for\ 1\ kg/year$$

Table S3 Fixed cost breakdown of A-CF production

Equipment	USD (April 2022)/kg of A-CF
Pre-treatment equipment	0.15
Melt-spinning machine	0.19
Stabilization oven	0.46
Carbonization oven	0.54
Post-processing equipment	0.31
Installation, commissioning	0.93
Drivers, rollers, ancillary, etc.	0.48
Overhead cost	0.34
Total	3.40

Table S4 Variable cost breakdown of A-CF production

Elements	Unit	Unit cost, USD	Amount required /kg of A-CF	USD/kg of A-CF
Precursor	kg	0.52[8]	2.01	1.05
Solvent (toluene)	kg	1.00[9]	0.52	0.52
Acid (40% HNO_3)	kg	0.82[10]	0.004	0.0032
Nitrogen	kg	0.53[11]	1.00	0.53
Electricity	kWh	0.072[12]	7.22	0.49
Miscellaneous (20%)	-	-	-	0.65
Total	-	-	-	3.24

A conversion factor of 0.80 is used to convert CAD to USD.

Table S5 Base case assumptions in the TEA study of A-CF production

Parameters	Value
Precursor cost ($/kg)	0.52
Solvent usage (kg/kg of CF)	26.00
Rate of solvent recovery (%)	98.00
Electricity consumption (kWh/kg of CF)	7.22
Electricity price ($/kWh)	0.072
Base Yield (%)	49.69
N_2 usage (kg/kg CF)	1.00
Capital cost ($/kg of CF)	3.40
WACC (%)	10.00
Yearly production (tonne/year)	2000

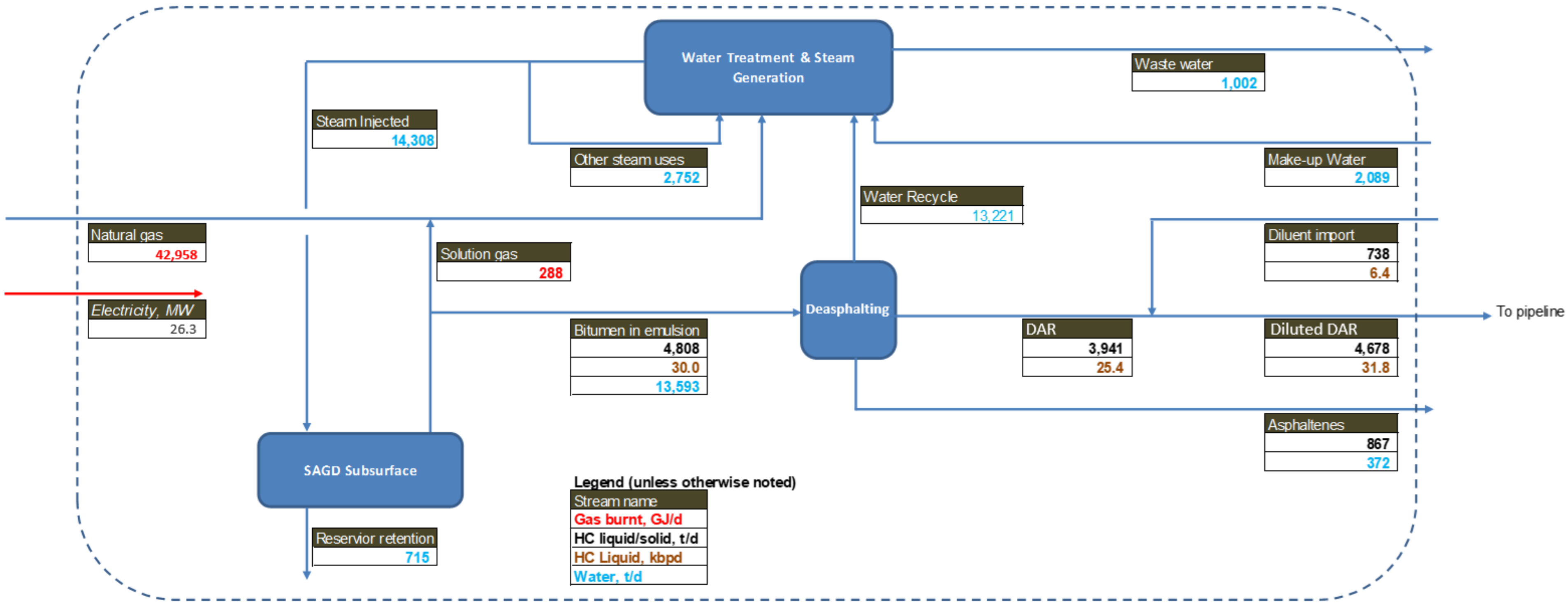

Fig. S1 Simplified mass and energy balance for the partial upgrading process of bitumen with steam assisted gravity drainage (SAGD). The data has been collected from a leading bitumen upgrading company in Alberta, Canada who has requested anonymity.

GWP For water (H_2O) extraction[13]

Underground water pumping energy = 0.45 kWh/m^3

Average treatment energy before supply = 0.327 kWh/m^3

Total energy = 0.78 kWh/m^3 = (0.78/1000) = $\frac{0.78\ kWh}{m^3} \times \frac{m^3}{1000\ kg}$ = 7.8x10^{-4} kWh/kg

EEF = 0.434 kg CO_2e/kWh

GWP for water treatment and supply = $\frac{0.00078\ kWh}{kg} \times \frac{0.434\ kg\ CO_2\!-\!eq}{kWh}$ = **3.39x10^{-4} kg CO_2-eq/kg H_2O**

Precursor energy calculation (i.e., upstream asphaltene extraction)

From Fig. S1, for per day basis,

Electricity input = 26.3 MW

Natural gas input = 42958 GJ/d = $\frac{42958\ GJ}{d} \times \frac{0.01157\ MW}{1\ GJ/d}$ = 497.02 MW

Total energy input = (497.02 + 26.3) MW = 523.32 MW = (523.22 × 24) MWh = 12559.8 MWh

Mass of produced asphaltene = 867 tonne

Mass of DAR = 3941 tonne

Allocation coefficient for asphaltene = $\frac{867}{867+3941}$ = 0.18

Allocated utility input for asphaltene = $\frac{12559.8\ MWh}{867\ tonne} \times \frac{0.18\times 1000\ kWh}{1\ MWh} \times \frac{1\ tonne}{1000\ kg}$ = 2.61 kWh/kg

Extraction energy for toluene (assuming the diluent as toluene) = 0.74 kWh/kg

Toluene required in the process = 738 tonne

Allocated embodied energy from toluene = $\frac{738\ tonne}{867\ tonne} \times \frac{0.18\times\ 0.74\ kWh}{kg} \times \frac{1\ tonne}{1000\ kg} \times \frac{1000\ kg}{1\ tonne}$ = 0.11 kWh/kg asphaltene

As water is recycled within the process, only energy for make-up water is considered.

Extraction energy for water = 7.8x10^{-4} kWh/kg

Make-up water required in the process = 2089 tonne

Allocated embodied energy from water = $\frac{2089\ tonne \times (7.8x10^{-4}) \times 0.18}{867\ tonne} \times \frac{1\ tonne}{1000\ kg} \times \frac{1000\ kg}{1\ tonne}$ = 0.0003 kWh/kg asphaltene

Total allocated upstream energy for extraction = (2.61 + 0.11 + 0.0003) kWh/kg = **2.73 kWh/kg asphaltene**

Table S6 Emission factors for specific midpoint indicators[14]

ILCD midpoint indicators	NG based without carbon capture and storage (CCS)	Hydropower
Climate change or Global Warming Potential, GWP (kg CO_2-eq / kWh)	0.434	0.0107
Freshwater eutrophication, FU (kg P-eq / kWh)	19.7E-06	1.33E-06
Acidification, AP (mol H^+-eq/kWh)	3.26E-04	4.45E-05
Ozone layer depletion, OLD (kg CFC-11-eq/kWh)	6.66E-08	2.37E-09

Table S7 Energy breakdown for the A-CF production technology

Process	Energy (kWh/kg asphaltene)	Energy (kWh/kg CF)*
Primary feedstock extraction	2.73	5.49
Pre-treatment & solvent recovery	2.16	4.35
Spinning	0.29	0.60
Acid treatment & stabilization	0.48	0.957
Carbonization	0.94	1.89
Balance of plant (BoP)	1.94	3.89
Total energy	8.53	17.19

*for baseline process yield of 49.67%

Table S8 GWP, FU, AP and OLD breakdown for the auxiliary feedstocks utilized in A-CF production technology

Feedstock	**Energy (kWh/kg CF)**	**GWP (kg CO_2-eq/kg CF)***	**FU (kg P-eq/kg CF)x10^{-4} #**	**AP (mol H^+-eq/kg CF) x10^{-3} ****	**OLD (kg CFC-11-eq/kg CF) ##**
Electricity	7.42	3.22	1.46	2.42	4.94
Heat	4.99	2.17	0.98	1.63	3.32
Toluene	4.57	1.98	0.90	1.49	3.04
N_2	0.19	0.003	0.037	0.062	0.13
HNO_3	0.0068	0.08	0.0013	0.002	0.005
Water	0.0038	0.0033	0.0007	0.001	0.003

*with a baseline emission factor = 0.434 kg CO_2-eq/kWh

#with a baseline emission factor = 19.7E-6 kg CO_2-eq/kWh

**with a baseline emission factor = 3.26E-4 kg CO_2-eq/kWh

##with a baseline emission factor = 6.66E-8 kg CO_2-eq/kWh

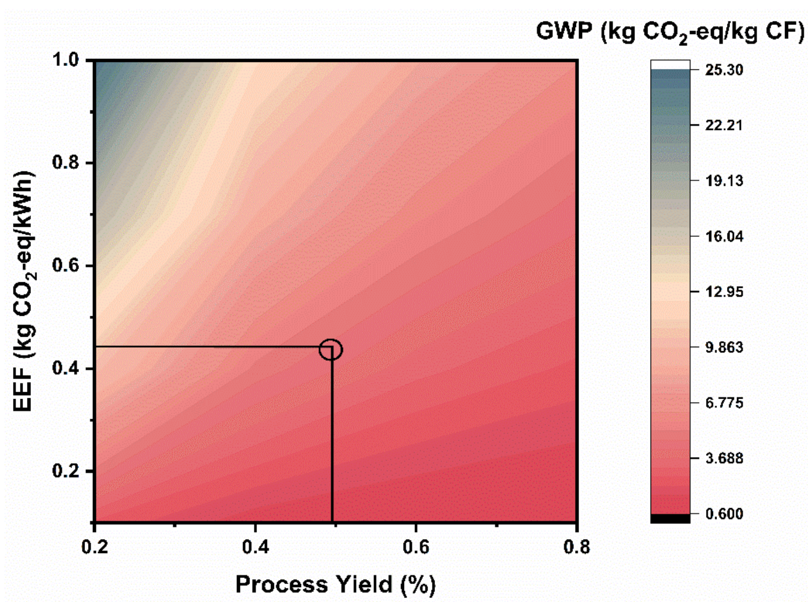

Fig. S2 Tandem or two-parameter sensitivity analysis for A-CF technology showing the effect of key performance indicators (electricity emission factor; EEF and process yield).

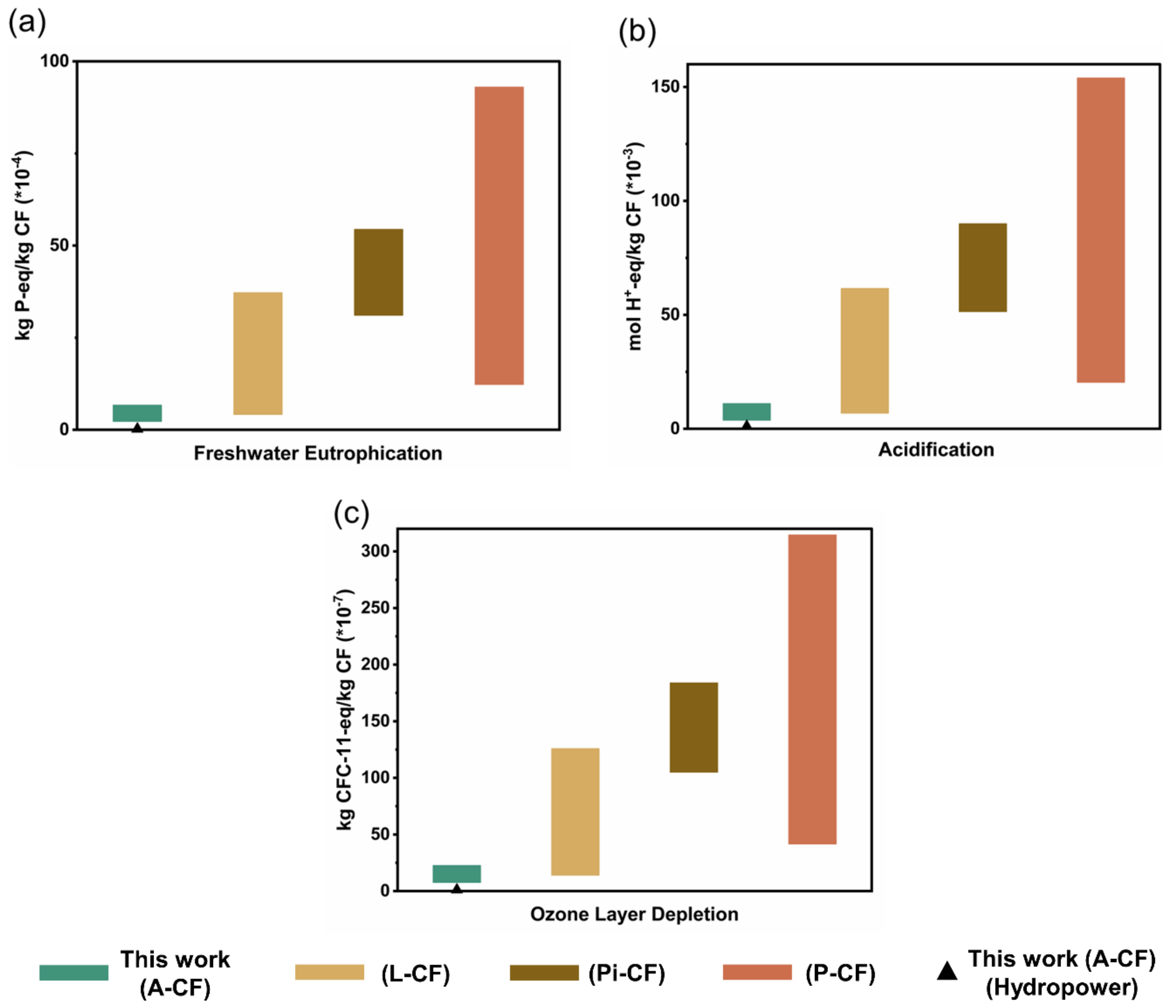

Fig. S3 Comparative cradle-to-gate assessment between different routes of CFPT, (a) freshwater eutrophication (FU), (b) acidification (AP), and (c) ozone layer depletion (OLD). The emission factors for base case as well as the low-carbon scenario are provided under Table S6. The low- and high-end range for A-CF have been derived from yield (25% vs 75%) while primary energy requirement for other incumbent routes have been collected from open literature (Table S9).

Table S9 Primary energy for the incumbent routes (data collected from open literatures)

	Energy (kWh/kg CF)	References
PAN based carbon fiber (P-CF)	83.33 – 472.22	[15,16]
	68.05	[17]
	79.44	[18]
	25.73	[19]
	195.56	[17,20]
	110.14	[21]
Lignin-based carbon fiber (L-CF)	188.89	[15]
	21.11	[22]
	186.12	[15]
Pitch-based carbon fiber (Pi-CF)	230	[16]
	276	[16,23]
	157.78	[24]

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