Supplementary Material

Carbon Dioxide Capture from Internal Combustion Engine Exhaust using Temperature Swing Adsorption

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Table A: Materials with lowest parasitic energies (PE) for CO_2 capture from coal flue gas [1]

Materials	PE, KJ/kg-CO_2
Mg-MOF-74	727
PPN-6-CH2TETA	*742*
mmen-CuBTTri	752
NaX	754
MgX	760
NaA	765
CaA	784
CaX	785
MgA	793
SIFSIX-3-Zn	805
ZIF-36-FRL	829
PPN-6-CH2TAEA	835
PPN-6-SO3Li	846
Zn-MOF-74	850

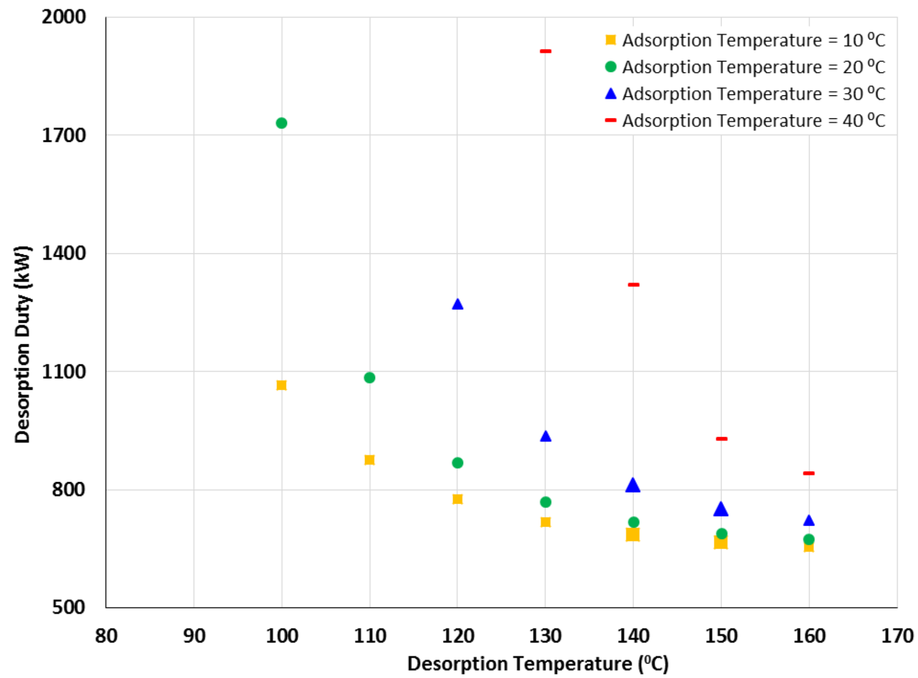


Figure A: Adsorption and desorption temperatures selection for PPN-6-CH2TETA [T_{ad} = 30 ^{0}C & T_{des} = 150 ^{0}C]

Table B: TSA model equations [2]

<table>
<tr><td>Component mass balance</td><td>$$\varepsilon_t \frac{\partial c_i}{\partial t} + \frac{\partial (u c_i)}{\partial z} + \rho_b \frac{\partial q_i}{\partial t} = 0$$</td><td rowspan="8">c = fluid phase conc. (mol/m^3)
u = superficial gas velocity (m/s)
q = solid phase conc. (mol/kg)
q^* = solid phase equilibrium conc. (mol/kg)
q^s = solid phase saturation conc. (mol/kg)
t = time (s)
z = vertical/height coordinate (m)
k = overall mass transfer coefficient (1/s)
C_g = heat capacity of gas (J/[K.m^3])
C_s = heat capacity of solid (J/[K.kg])
C_{ads} = adsorbed phase heat capacity (J/[K.kg])
ΔH = heat of adsorption (J/mol)
h_L = heat transfer coefficient (J/m^2.s.K)
D = column inner diameter (m)
p = fluid pressure (Pa)
d_p = particle diameter (m)
K = Henry coefficient (mol/[kg.Pa])
R = ideal gas constant (J/K.mol)
T = temperature (K)
T_{amb} = ambient temperature (K)
H_{ads} = heat of adsorption (J/mol)
A = area (m^2)
$Q_{v,f}$ = volumetric feed flow rate (m3/s)
m_f = feed mass flow rate (kg/s)
y = component mass fraction
L = bed height (m)
μ = dynamic viscosity (kg/[m.s])
ρ = fluid phase density (kg/m^3)</td></tr>
<tr><td>Overall mass balance</td><td>$$\varepsilon_t \frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial z} + \rho_b \sum_{j=1}^{N} \frac{\partial q_j}{\partial t} = 0$$</td></tr>
<tr><td>Mass transfer</td><td>$$\frac{\partial q_i}{\partial t} = k_i (q_i^* - q_i)$$</td></tr>
<tr><td>Energy balance</td><td>$$\left(\varepsilon_t C_g + \rho_b C_s + \rho_b C_{ads}\right) \frac{\partial T}{\partial t} + u C_g \rho \frac{\partial T}{\partial z} - \rho_b \sum_{j=1}^{N} \left(-\Delta H_j\right) \frac{\partial q_j}{\partial t} + \frac{h_L}{D}(T - T_{media}) = 0$$</td></tr>
<tr><td>Momentum balance (Ergun equation)</td><td>$$\frac{\partial p}{\partial z} = -\frac{150\mu(1-\varepsilon_b)^2}{\varepsilon_b^3 d_p^2} u - \frac{1.75(1-\varepsilon_b)\rho}{\varepsilon_b^3 d_p} |u| u$$</td></tr>
<tr><td>q equilibrium & K calculations</td><td>$$q_i^*(q_i^s + K_i C_i RT)) - q_i^s K_i C_i RT = 0$$
$$K_i - K_i^{ref} e^{\left[-\frac{H_i^{ads}}{R\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)}\right]} = 0$$</td></tr>
<tr><td>Bed area & feed flow rate</td><td>$$A = \frac{\pi D^2}{4}$$
$$Q_{v,f} = \frac{m_f}{\rho}$$</td></tr>
<tr><td>Auxiliary relationships</td><td>$$\sum_{j=1}^{N} y_j = 1$$
$$c_i = y_i * \frac{p}{RT}$$
$$p - \sum_{j=1}^{N} C_j RT = 0$$</td></tr>
</table>

	$$c_{tot} = \sum_{j=1}^{N} C_j$$	ρ_b = bed density (kg/m^3) ε_t = overall void fraction ε_b = bed void fraction i = component number N = total number of components *ref* = reference, *tot* = total
Initial and boundary conditions for adsorption	$$y_{CO2}\|_{z=0} = y_{CO2,feed}$$ $$T\|_{z=0} = T_{feed}$$ $$y_{CO2}\|_{z=L} = y_{CO2,residue}$$ $$\left.\frac{\partial T}{\partial z}\right\|_{z=1} = 0,\ \left.\frac{\partial c}{\partial z}\right\|_{z=1} = 0,\ \left.\frac{\partial P}{\partial z}\right\|_{z=1} = 0$$	
Parameters values	D = 0.25 m, d_p = 0.003 m, h_L = 3000 (J/m^2.s.K), k = 0.3 (1/s) L = 1 (m), T_{feed} = 303 (K), T_{amb} = 293 (K), ε_b= 0.4, ε_t = 0.742	

Table C: PPN-6-CH2TETA parameters values [1].

Material's Parameter	Value
Heat of adsorption for CO_2 (kJ/mol), H_{ads}	-48.23
Heat of adsorption for N_2 (kJ/mol), H_{ads}	-18.29
Henry coefficient for CO_2 (mol/kg.Pa), K_{ref}	0.00652
Henry coefficient for N_2 (mol/kg.Pa), K_{ref}	6.99e-07
Saturation loading for CO_2 (mol/kg), q^s	4.77
Saturation loading for N_2 (mol/kg), q^s	0.04
Density (kg/m3), ρ_b	883.8
Heat capacity (J/kg.K), C_s	985

- In this study, N_2 and O_2 co-adsorption has not been considered. For the modeling/simulation purpose, O_2 is considered as N_2.
- The adsorbent material was assumed to be fully regenerated prior to every adsorption step. This assumption is reasonable for Case 1 (desorption in parking lot). For Cases 2 & 3, the adsorbent material cannot be fully regenerated, and a small fraction of CO_2 will remain in the adsorbent material before the start of a new TSA cycle.
- The adsorption model has been solved, until 90% CO_2 presents in the fresh feed is captured by the material. The CO_2 capture rate decreases with increase in the adsorption time.
- Percentage CO_2 capture rate is calculated, as: (total inlet CO_2 – total outlet CO_2)/total inlet CO_2×100. Total inlet CO_2 and total outlet CO_2 are calculated by integrating/summing inlet CO_2 to the bed and outlet CO_2 from the bed, for entire adsorption time.
- For a specific feed flow rate and composition, heat of adsorption is calculated using total heat removed and amount of CO_2 attached to the material.
- In this study, detailed heat exchange inside the adsorption bed has not been studied.

Exergy Calculations for 1 liter Diesel [3, 4]

1. Diesel fuel:

$\varepsilon_{1,f}$ = 1.0338*LHV = 38.53 MJ [LHV = 37.27 for 1 liter diesel]

2. Mechanical power:

$\varepsilon_{1,mp}$ = 13.05 MJ

3. Engine cooling:

$\varepsilon_{1,ec} = Q \times (1-T0/T) = 10.02 \times (1 - 298/393) = 2.42$ MJ [T = 393 K]

4. Engine exhaust:

$\varepsilon_{1,ee} = Q \times (1-T0/T) = 8.24 \times (1 - 298/524.4) = 3.56$ MJ [T = 524.4 K: log mean of 773 and 338.3 K]

$\varepsilon_{2,ee} = Q \times (1-T0/T) = 5.97 \times (1 - 298/316.8) = 0.35$ MJ [T = 316.8 K: log mean of 338.3 and 298 K]

5. Cooling and adsorption:

$\varepsilon_{1,ca} = Q \times (1-T0/T) = 3.96 \times (1 - 298/358.6) = 0.67$ MJ [T = 358.6 K: log mean of 423 and 303 K]

$\varepsilon_{2,ca} = Q \times (1-T0/T) = 4.21 \times (1 - 298/303) = 0.07$ MJ [T = 303 K]

6. Heating and desorption:

$\varepsilon_{1,hd} = - Q \times (1-T0/T) = - 3.74 \times (1 - 298/358.6) = - 0.63$ MJ [T = 358.6 K: log mean of 303 and 423 K]

$\varepsilon_{2,hd} = - Q \times (1-T0/T) = - 4.21 \times (1 - 298/423) = - 1.24$ MJ [T = 423 K]

7. Inter-stage CO_2 cooling:

$\varepsilon_{1,is} = Q \times (1-T0/T) = 0.22 \times (1 - 298/358.6) = 0.04$ MJ [T = 358.6 K: log mean of 423 and 303 K]

$\varepsilon_{2,is} = Q \times (1-T0/T) = 0.45 \times (1 - 298/403.6) = 0.12$ MJ [T = 403.6 K: log mean of 527.4 and 303 K]

$\varepsilon_{3,is} = Q \times (1-T0/T) = 0.42 \times (1 - 298/401.1) = 0.11$ MJ [T = 401.1 K: log mean of 518.4 and 305 K]

$\varepsilon_{4,is} = Q \times (1-T0/T) = 0.52 \times (1 - 298/300.6) = 0.004$ MJ [T = 300.6 K: log mean of 305 and 298 K]

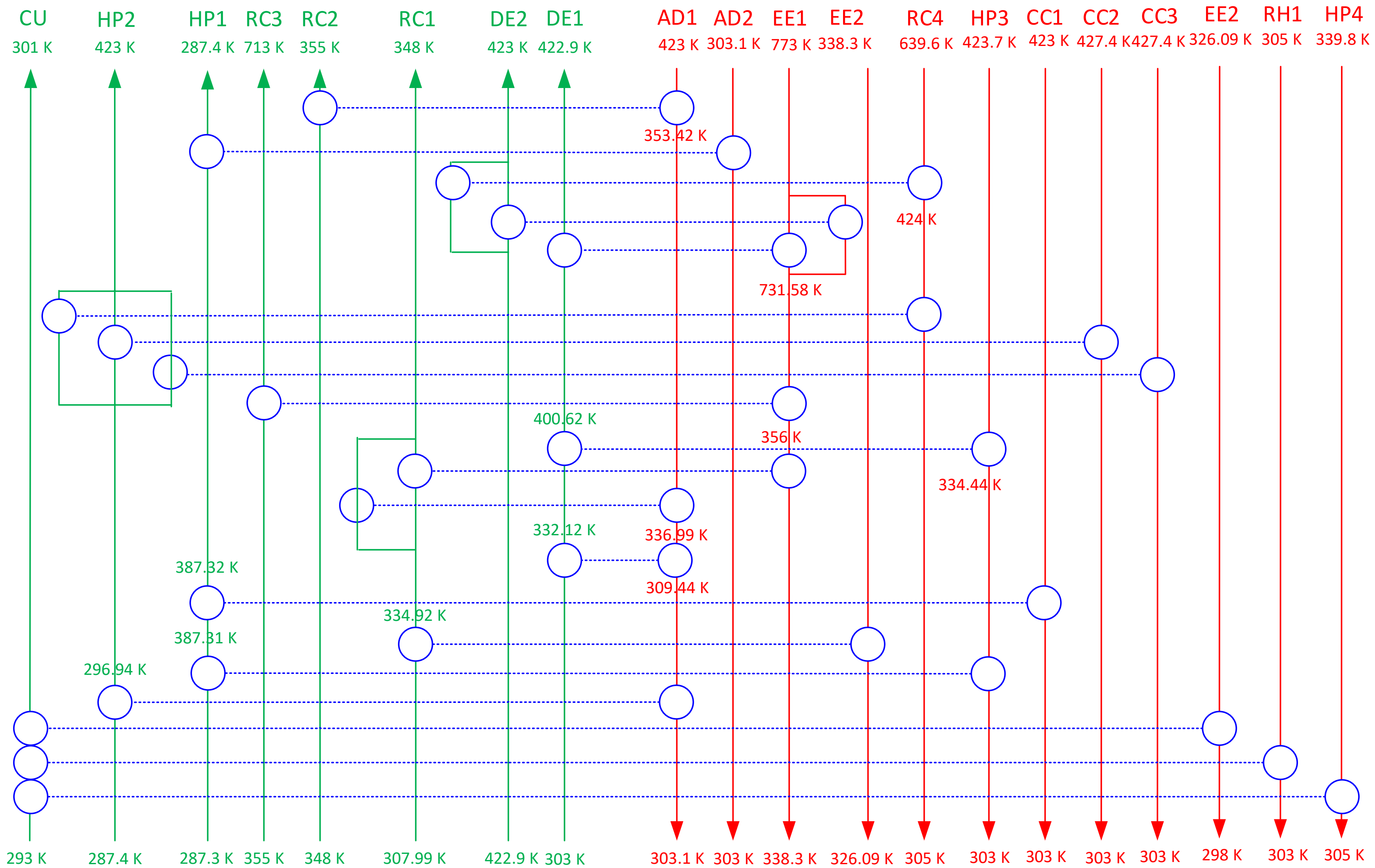
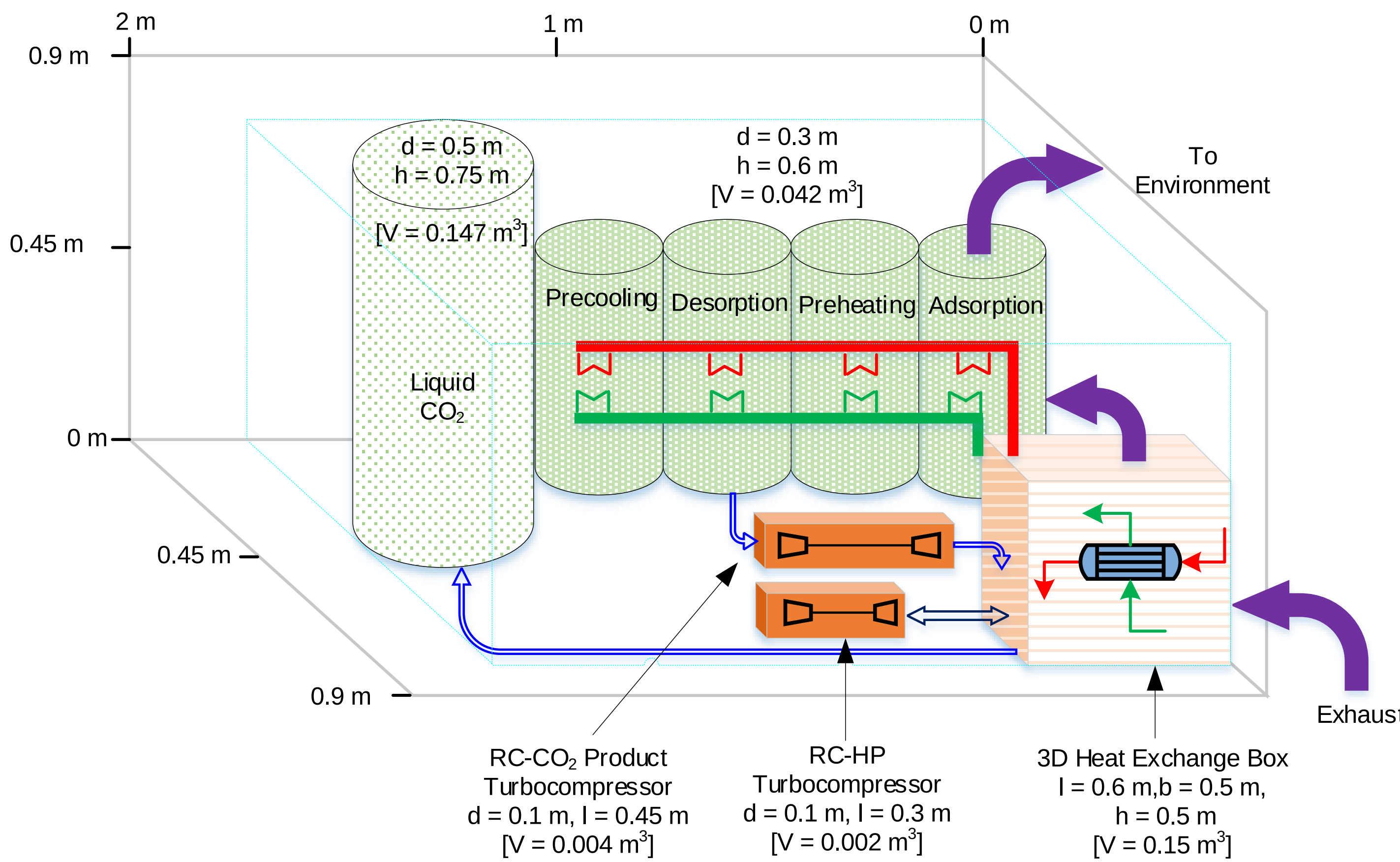


Figure B: Grid representation of heat exchanger network



Space over truck cabin = 2 m × 0.9 m × 0.9 m

Space required by CO_2 capture system = 1.7 m × 0.8 m × 0.75 m

Space required by CO_2 capture system without CO_2 tank = 1.2 m × 0.8 m × 0.6 m

Figure C: Estimated volume of the CO_2 capture and storage system for delivery truck (size of turbocompressor is estimated based on Casey et al. [5]; Volume of 3D heat exchange box is estimated with 100 m^2/m^3 surface area to volume ratio)

Table D: Conversion of 1 kg of CO_2 into green fuels [6]

	Methane	**Methanol**	**DME**	**Gasoline**
Fuel, kg	0.37	0.67	0.46	0.26
Electricity consumptions, MJ	24.5	20.5	21.3	18.8
Photovoltaic panels area (Switzerland), m^2	7.1	5.9	6.2	5.4

Table E: Weight, payload and diesel consumption for different vehicles

	Weight (kg)	Payload (kg)	Diesel Used per 100 km, l	Diesel Used & CO_2 produced in 250 km Travel				References
				Diesel Used, l	Product CO_2, kg	Product CO_2, l	Storage Tank, kg	
Car	1678	454	6.5	16.25	34.29	48.09	34.62	7, 8, 16
SUV	1746	680	11	27.5	58.03	81.38	58.59	7, 8, 16
Pickup Truck	2563	1678	13	32.5	68.58	96.18	69.25	7, 8, 16
Van/Minibus	3708	2381	11	27.5	58.03	81.38	58.59	7, 8, 16
School Bus	5897	5216	22	55	116.05	162.76	117.19	7, 8, 16
City Bus	5897	8391	58	145	305.95	429.09	308.95	7, 8, 16
City Hybrid Bus	5897	8391	45	112.5	237.38	332.92	239.70	7, 8, 16
City Delivery	4423	3946	21.2	53	111.83	156.84	112.93	7, 9, 16
Regional Delivery Truck	6500	5500	22.2	55.5	117.11	164.24	118.25	9, 16
Long Haul Tractor Trailer	14400	25600	36.2	90.5	190.96	267.81	192.83	9, 16
Small Tanker	1.1×10^7	4.6×10^7	3124	7810	16479.10	23111.94	16640.60	10, 16
Ferry	8.0×10^6	5.853×10^5	5151	12877.5	27171.53	38108.06	27437.81	11, 16
Cruise ship	1.0×10^8	7.92×10^5	23463	58657.5	123767.33	173583.67	124980.24	12, 16
Train	4.5×10^5	5.77×10^5	282.73	707	1491.40	2091.69	1506.02	13-16

Table F: Percent added weight of CO_2 capture system and liquid storage (CCS-LS) with respect to total weight and payload of different vehicles (M_{AD}, V_{AD}: mass and volume of adsorbent)

	Travel Time	Diesel Used per hour, l	Product CO_2 per hour, kg	M_{AD}, kg	V_{AD}, l	CCS-LS Weight, kg	CCS-LS Volume, l	CCS-LS Weight / Payload	CCS-LS Weight / Total Weight
Car	4	4.06	8.57	85.72	106.48	154.63	154.57	34.06	7.25
SUV	4	6.88	14.51	145.06	180.20	261.68	261.58	38.48	10.79
Pickup Truck	4	8.13	17.14	171.44	212.97	309.26	309.14	18.43	7.29
Van/Minibus	8	3.44	7.25	72.53	90.10	189.15	171.48	7.94	3.11
School Bus	8	6.88	14.51	145.06	180.20	378.30	342.96	7.25	3.40
City Bus	8	18.13	38.24	382.44	475.08	997.34	904.17	11.89	6.98
City Hybrid Bus	8	14.06	29.67	296.72	368.59	773.80	701.51	9.22	5.42
City Delivery	8	6.63	13.98	139.79	173.65	364.54	330.49	9.24	4.36
Regional Delivery Truck	4	13.88	29.28	292.76	363.68	528.12	527.92	9.60	4.40
Long Haul Tractor Trailer	4	22.63	47.74	477.39	593.03	861.17	860.84	3.36	2.15
Small Tanker	14	557.86	1177.08	11770.79	14622.09	44890.48	37734.03	0.10	0.08
Ferry	8	1609.69	3396.44	33964.41	42191.81	88573.74	80299.87	15.13	1.03
Cruise ship	8	7332.19	15470.92	154709.16	192185.29	403456.73	365768.96	50.94	0.40
Train	4	176.71	372.85	3728.50	4631.68	6725.92	6723.37	1.17	0.65

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