Supplementary Material

Choosing a liquid hydrogen carrier for sustainable transportation

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Renewable dimethyl ether (DME) cost in Table 3

Calculating the DME production cost for comparison in **Tab. 3** in the manuscript. DME case uses double the H_2 requirement of MeOH and is assumed to use less non-H_2 energy requirements due to the greater one-step exothermicity of the DME reaction. **Table S-1** calculates this non-H_2 energy difference and **Table S-2** computes the DME cost to use in the reforming analysis. Identifiers of each parameter are used to show the calculation steps.

***Supplementary Table 1**: DME production cost without H_2*

Parameter	Identifier	Value	Units	Equation
Basis	MeOH1	*1.0*	kg_{MeOH}	input
MeOH H_2 stoic.	MeOH2	*0.126*	$kg_{H2}\ kg_{MeOH}^{-1}$	input
Basis	DME1	*1.0*	kg_{DME}	input
DME H_2 stoic.	DME2	*0.131*	$kg_{H2}\ kg_{DME}^{-1}$	input
MeOH H_2 cost %	MeOH3	*80*	% of total cost	Input, data from [1]
MeOH non-H_2 cost %	MeOH4	*20*	% of total cost	input, data from [1]
MeOH Prod. w/o H_2	MeOH5	2.1	$MWh\ tonne_{MeOH}^{-1}$	= MeOH4 * MeOH7
MeOH Prod. w/o H_2	MeOH6	16.7	$MWh\ tonne_{H2}^{-1}$	= MeOH5 * (MeOH1/MeOH2)
DME Prod. w/o H_2	DME4	1.2	$MWh\ tonne_{DME}^{-1}$	= DME6 - MeOH7 * MeOH3 * 2
DME Prod. w/o H_2	DME5	9.1	$MWh\ tonne_{H2}^{-1}$	= DME4 * (DME1/DME2)

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***Supplementary Table 2**: DME production cost with H_2*

Parameter	Identifier	Value	Units	Equation
MeOH Prod. energy	MeOH7	*10.3*	MWh $tonne_{MeOH}^{-1}$	input, data from [1]
DME Prod. energy	DME6	*18.0*	MWh $tonne_{DME}^{-1}$	input
MeOH Prod. cost	MeOH8	*1.45*	\$ kg_{MeOH}^{-1}	Input – Case A, data from [1]
MeOH Prod. cost	MeOH9	11.5	\$ $kg_{H2equiv}^{-1}$	= MeOH8 * (MeOH1/MeOH2)
DME Prod. cost	DME7	2.6	\$ kg_{DME}^{-1}	= DME8 * (DME2/DME1)
DME Prod. cost	DME8	20.1	\$ $kg_{H2equiv}^{-1}$	= MeOH9 * MeOH3 * 2 + (DME5/MeOH6) * MeOH8 * MeOH4 * (MeOH1/MeOH2)

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RC&C cost as a function of carbon tax (Fig. 4B data)

***Supplementary Table 3**: ICEV emissions with example US$ 30 mt_{CO2}^{-1} carbon tax*

Parameter	Identifier	Value	Units	Equation
Vehicle miles per gallon gas	GAS1	*24-30*	miles per US gallon (MPG)	
Vehicle efficiency gas fuel	GAS2	*40*	%	
Vehicle efficiency MeOH fuel	MeOH1	*45*	%	
Total mileage	VEHIC1	*250000*	km	
Average speed	VEHIC2	*80*	km hr^{-1}	
Total driving hours	VEHIC3	3125	hrs	=VEHIC1/VEHIC2
Vehicle size	VEHIC4	62.0	kW	=GAS7/VEHIC3
Vehicle avg miles per gallon gas	GAS3	27.0	Avg. MPG	=AVERAGE(GAS1)
Vehicle Km per liter gas	GAS4	11.5	km L^{-1}	=GAS3*1.609/3.785
Gasoline Lower heating value	GAS5	*8.9*	kWh L^{-1}	
Gasoline Joule per Km	GAS6	0.8	kWh km^{-1}	=GAS5/GAS4
Total kWh Gasoline	GAS7	193834	kWh	=VEHIC1*GAS6
Methanol Lower heating value	MeOH2	*5.54*	kWh kg^{-1}	
Total fuel mass	MeOH3	31101	kg MeOH	=GAS7/MeOH2*GAS2/MeOH1
Total CO2 emissions	MeOH4	42717	kg CO_2	=MeOH3*1000/(32.042) * (12.011+2*15.9994)/1000
Carbon tax	CT1	*30*	US$ mt^{-1} CO_2	
Lifetime emission cost	MeOH_CT2	1281.5	US$ $lifetime^{-1}$	=MeOH4/1000*CT1
Lifetime CO2 per 100 km	MeOH_CT3	0.513	US$ CO_2 100 km^{-1}	=MeOH_CT2/(VEHIC1/100)

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***Supplementary Table 4**: FCV emissions with example US$ 30 mt_{CO2}^{-1} carbon tax*

Parameter	Identifier	Value	Units	Equation
Vehicle efficiency H2 fuel	H2_1	*90*	%	
H2 Lower heating value	H2_2	*33.30*	kWh kg^{-1}	
Total fuel mass	H2_3	3107	kg H_2	=GAS7/H2_2 * GAS2/H2_1
Lifetime RC&C cost 2020	H2_4	-8	US$ $lifetime^{-1}$	=US$ kWh^{-1} (RC&C 2020 **Table S-6**) * GAS7
RC&C eqv H2 cost 2035	H2_2035	0.00	US$ kg_{H2}^{-1}	Input for **Table S-7**
Lifetime RC&C cost 2035	H2_4	8439	US$ $lifetime^{-1}$	= US$ kWh^{-1} (RC&C 2035 **Table S-6**) * GAS7
RC&C eqv H2 cost 2035	H2_2035	2.72	US$ kg_{H2}^{-1}	Input for **Table S-7**
Lifetime RC&C cost 2050	H2_5	10734	US$ $lifetime^{-1}$	= US$ kWh^{-1} (RC&C 2050 **Table S-6**) * GAS7
RC&C eqv H2 cost 2050	H2_2050	3.45	US$ kg_{H2}^{-1}	Input for **Table S-7**

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***Supplementary Table 5**: Emissions tax on ICEV as a function of carbon tax*

Parameter	Identif.	Values						Units	Equation
Carbon tax	CT_1	*0*	*30*	*50*	*100*	*250*	*500*	US$ $mtCO_2^{-1}$	
Lifetime CO2 per 100 km	CT_2	**0.00**	**0.51**	**0.85**	**1.71**	**4.27**	**8.54**	US$ CO_2e $100\ km^{-1}$	MeOH_CT3 from **Table S-3**
Lifetime emission amount	CT_3	Na	**1282**	**2136**	**4272**	**10679**	**21358**	US$ CO_2 $lifetime^{-1}$	For example, US$ 30 mt_{CO2}^{-1} is MeOH_CT2 from **Table S-3**
Tax on ICEV emissions	CT_4	0.0	20.7	34.4	68.9	172.2	344.3	US$ kW^{-1}	=CT_3/VEHIC4 Input for **Table S-6**

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***Supplementary Table 6**: Emissions tax on ICEVs as a function of carbon tax, component costs of FCVs derived from Share %, this example is for US$ 30 mt_{CO2}^{-1} carbon tax*

Vehicle and Component	Component cost	Units	Share, %	US$ kWh^{-1}	Equation
ICEV					
Drivetrain	*21.0*	US$ kW^{-1}	7.7%	0.007	
Emissions	*272.7*	US$ kW^{-1}	92.8%	0.087	Add CT_4 from **Table S-5** here
SUM	293.7	US$ kW^{-1}	100.6%	0.094	
PEMFCV	2020				
Drivetrain	173.6	US$ kW^{-1}	*59.1%*	0.056	Share % same as **Fig. 4A**
Emissions	120.2	US$ kW^{-1}	*40.9%*	0.038	
R&C	-0.1	US$ kW^{-1}	*0.0%*	0.000	
SUM	293.7	US$ kW^{-1}	*100.0%*	0.094	Sum matches ICEV case
PEMFCV	2035				
Drivetrain	60.2	US$ kW^{-1}	*20.5%*	0.019	Share % same as **Fig. 4A**
Emissions	120.2	US$ kW^{-1}	*40.9%*	0.038	
R&C	113.3	US$ kW^{-1}	*38.6%*	0.036	
SUM	293.7	US$ kW^{-1}	*100.0%*	0.094	Sum matches ICEV case
PEMFCV	2050				
Drivetrain	29.4	US$ kW^{-1}	*10.0%*	0.009	Share % same as **Fig. 4A**
Emissions	120.2	US$ kW^{-1}	*40.9%*	0.038	
R&C	144.1	US$ kW^{-1}	*49.1%*	0.046	
SUM	293.7	US$ kW^{-1}	*100.0%*	0.094	Sum matches ICEV case

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Supplementary Table 7**: Derived RC&C Cost for **Fig. 4B

Carbon Tax, US$ mt_{CO2}^{-1}	RC&C 2020, US$ kg_{H2}^{-1}	RC&C 2035, US$ kg_{H2}^{-1}	RC&C 2050, US$ kg_{H2}^{-1}
0	**-0.28**	**2.44**	**3.18**
30	**0.00**	**2.72**	**3.45**
50	**0.18**	**2.90**	**3.64**
100	**0.64**	**3.36**	**4.10**
250	**2.03**	**4.75**	**5.49**
500	**4.34**	**7.06**	**7.79**

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References

1. Tountas AA, Peng X, Tavasoli A V., Duchesne PN, Dingle TL, Dong Y, et al. Towards Solar Methanol: Past, Present, and Future. Advanced Science. 2019;6(8):1–52.