Supporting information for:

Strategies for low temperature Liquid Organic Hydrogen Carrier dehydrogenation

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Preheating

Substance properties & reaction parameters

conversion	0.8	±	0.1	kJ mol(H_2)$^{-1}$	
c_P of	1.91	±	0.02	J g^{-1} K^{-1}	
H18-DBT	518.97	±	5.19	J mol^{-1} K^{-1}	
$T_{ambient}$	293.15	K			
$T_{reaction}$	473.15	K			
$Q_{preheating}$	12.97	±	1.61	kJ mol(H_2)$^{-1}$	*no heat recovery*
	0.72	±	7.2E-03		*heat recovery with Δ T=10K*

Heat of reaction

$\Delta^R h$	65.39	±	1.05	kJ mol(H_2)$^{-1}$	*at standard conditions*
	68.97	±	1.06		*at 200 °C*

Heat loss to surroundings

P_{system}	10			kW_{LHV}
LHV(H_2)	241.9			kJ mol(H_2)$^{-1}$
$P_{ambient}$	0.5	±	0.1	$kW_{thermal}$
$P_{ambient}$	12.10	±	2.42	kJ mol(H_2)$^{-1}$

Provision of low pressure

$P_{surrounding}$ 1 bar P_{system} 0.1 bar T 473.15 K

vaccum pump

$P_{pump,Carnot}$	9.06			kJ mol(H_2)$^{-1}$
$P_{pump,low}$	17.84			kJ mol(H_2)$^{-1}$
$P_{pump,average}$	58.08	±	57.94	kJ mol(H_2)$^{-1}$

eletrochemical compression

U_{min}	0.05	V
$U_{polarization}$	*negligible*	
U_{ohmic}	0.05	V
U_{actual}	0.09	V
E_{actual}	18.12	kJ mol(H_2)$^{-1}$

For comparison: values for electrochemical compression reported by Rohland et al.

min		max	
0.25	-	0.35	kWh / Nm³
900	-	1260	kJ / Nm³
20.17	-	28.24	kJ mol(H_2)$^{-1}$

Ströbel et al. - Fig. 7; https://www.sciencedirect.com/science/article/pii/S0378775301009417
ca. 0.13 V

Purification - removal of inert gas/vapor

inert gas (CO_2)

compare: Müller et al., 2017, Hydrogen Storage in Formic Acid: A Comparison of Process Options

	average			lowest value in literature	accepted range		
				kJ mol^{-1}(CO_2)			
PSA	113.7	±	167.0	4.0	20	-	100
TSA	213.4	±	96.2	105.6	105	-	200
amine scrubbing	167.2	±	52.2	31.7	80	-	200
cryogenic	113.3	±	26.4	95.0	95	-	120
				kJ mol^{-1}(H_2)			
PSA	1023.4	±	1502.7	36	180	-	900
TSA	1921.0	±	866.2	950.4	945	-	1800
amine scrubbing	1504.9	±	469.68	285.3	720	-	1800
cryogenic	1019.5	±	237.21	855	855	-	1080

analogously to Hydrogen Storage in Formic Acid: A Comparison of Process	21.7	kJ mol(CO_2)$^{-1}$
	195.3	kJ mol(H_2)$^{-1}$

inert vapor

assumption for condensable inert substance: n-decane (T_{boil}=174,1°C)

T	174.1	°C
$\Delta_{vap}h$	38.8	kJ mol(decane)$^{-1}$
	348.9	kJ mol(H_2)$^{-1}$

assumption for condensable inert substance: n-hexane (T_{boil}=69°C)

T	69.0	°C
$\Delta_{vap}h$	27.4	kJ mol(hexane)$^{-1}$
	246.2	kJ mol(H_2)$^{-1}$

LOHC

removal of LOHC vapor from the H_2 stream
removal of LOHC vapor by condensation; cooling is possible against ambient or by preheating the cold inlet stream
--> no energy demand needed

Energy demand for evaporation

$\Delta^{vap}h$(H18-DBT)	88.2	±	1.5	kJ mol(LOHC)$^{-}$	at 373.47 K
T	473.15	K			
$\Delta^{vap}h$(H18-DBT)	65.79	±	1.50	kJ mol(LOHC)$^{-1}$	
	7.31	±	0.17	kJ mol(H_2)$^{-1}$	

enthalpy of evaporation relative to enthalpy of reaction
10.60%
enthalpy of evaporation relative to lower heating value
3.02%

$\Delta^{vap}h$(H0-BT)	73.3	±	3	kJ mol(LOHC)$^{-1}$	at 298.15 K
	12.22	±	0.5	kJ mol(H_2)$^{-1}$	

enthalpy of evaporation relative to enthalpy of reaction
17.71%
enthalpy of evaporation relative to lower heating value
5.05%

Waste heat of a fuel cell (η=50%)	121.0

Scenario: Dehydrogenation at 100 mbar (low pressure by vacuum pump)

preheating	0.7	±	0.0	*heat recovery with ΔT=10K*
preheating	13.0	±	1.6	*no heat recovery*
enthalpy of reaction	69.0	±	1.1	
heat loss to surroundings	12.1	±	2.4	
vacuum pump	58.1	±	57.9	+ purification
Σ	**152.1**	±	**58.0**	

Scenario: Dehydrogenation at 100 mbar (low pressure by ECC)

preheating	0.7	±	0.0	*heat recovery with ΔT=10K*
preheating	13.0	±	1.6	*no heat recovery*
enthalpy of reaction	69.0	±	1.1	
heat loss to surroundings	12.1	±	2.4	
ECC	18.1	±	1.8	
Σ	**112.2**	±	**3.6**	
heat	94.0	±	3.1	
			14.98%	

Scenario: Reactive distillation

preheating	0.7	±	0.0	
preheating	13.0	±	1.6	
enthalpy of reaction	69.0	±	1.1	
Evaporation	12.2	±	0.5	
Vaporisation relative to feed flow	1.0			+ purification & vaccum pump
Σ	**94.2**	±	**2.0**	

Scenario: Dilution with hexane down to a partial pressure of 100 mbar

preheating	0.7	±	0.0
preheating	13.0	±	1.6
enthalpy of reaction	69.0	±	1.1
Evaporation	246.2	±	
Σ	**328.2**	±	**1.9**

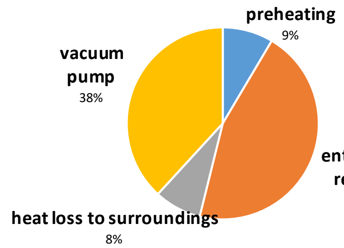

Figure S1 Shares on energy demand for the low pressure option (Mechanical vacuum pump)

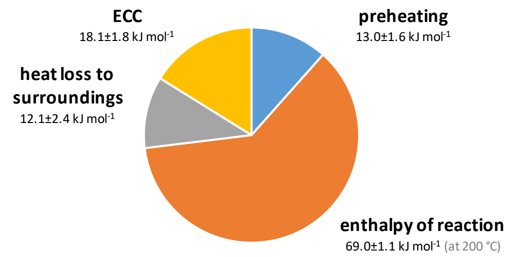

Figure S2 Shares on energy demand for the low pressure option (electrochemical compression)