Supporting Information

Alcohol-Based Adsorption Heat Pumps using Hydrophobic Metal-Organic Frameworks

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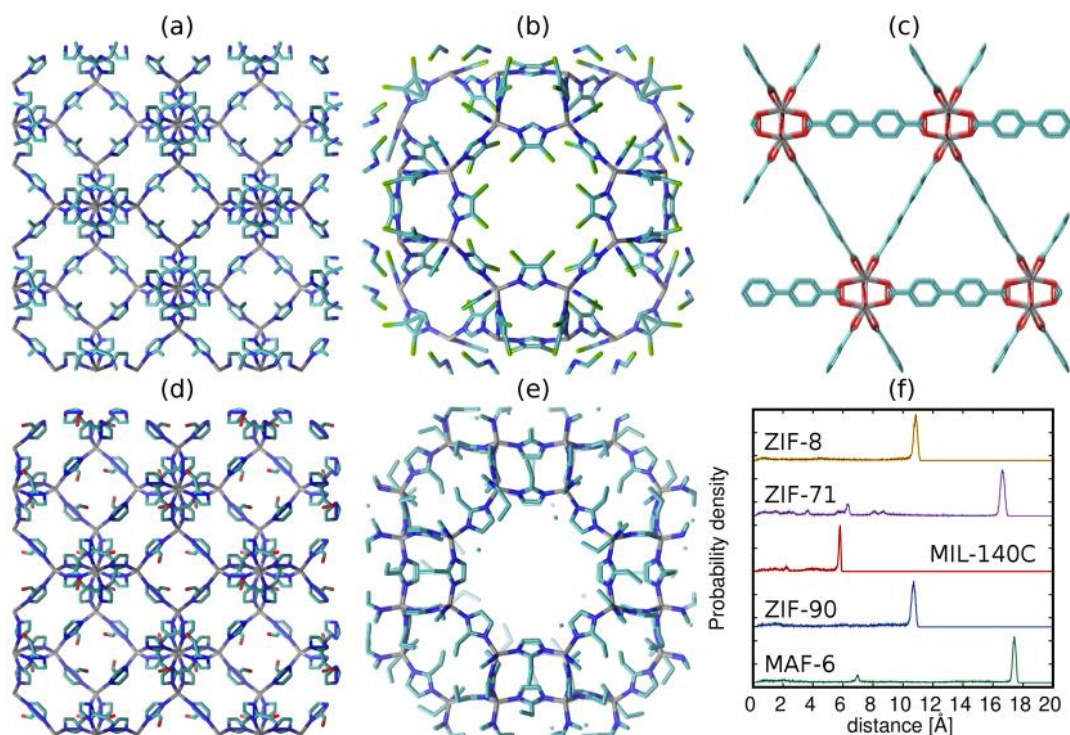
Figure S1. Schematic representation of the framework connectivity of (a) ZIF-8, (b) ZIF-71, (c) MIL-140C, (d) ZIF-90 and (e) MAF-6. (f) Pore Size Distribution. Nitrogen atoms are coloured in blue, carbon atoms in cyan, oxygen atoms in red, chlorine atoms in green, and zirconium and zinc atoms in grey. Hydrogen atoms are omitted for clarity.

Table S1. Structural properties of the selected MOFs, density, pore volume, helium void fraction, surface area, and pore size. Experimental values [1-3] are included between parentheses for comparison.

MOF	Topology	ρ [kg m^{-3}]	V_P [cm^{3}g^{-1}]	HvF	S_A [m^{2}g^{-1}]	Pore Size [Å]
ZIF-8	SOD	924.586	0.52 (0.685)[1]	0.484	1732.4 (1696)[1]	10.8
ZIF-90	SOD	988.431	0.51 (0.485)[1]	0.507	1661.3 (1280)[1]	10.7
ZIF-71	RHO	1154.904	0.42 (0.385)[1]	0.496	1379.2 (1183)[1]	16.6
MAF-6	RHO	813.579	0.59 (0.61)[2]	0.482	1664.4 (1695)[2]	17.4
MIL-140C	-	1173.139	0.34 (0.36)[3]	0.400	1298.9 (-)	5.8

MOF	Atom	Partial Charge [e]
ZIF-8		
	N1	-0.4973
	Zn1	1.022
	C1	0.4958
	C2	-0.0672
	C3	-0.272
	H2	0.1023
	H3	0.0632
ZIF-71		
	N1	-0.2873
	Zn1	1.2054
	Cl1	-0.24505
	C1	0.14155
	C3	0.16585
	H1	-0.01125
MIL-140C		
	O1	-0.6152887
	O2	-0.3996415
	Zr	1.50139
	C1	0.370644
	C2	-0.107838
	C3	0.023914
	C4	0.0630835
	C5	0.0203093
	H3	0.0348988
	H4	0.04140775
ZIF-90		
	C1	0.3078
	C2	-0.0255
	C3	-0.4335
	H1	0.0321
	H2	0.2944
	N1	-0.3229
	O1	-0.1371
	Zn1	1.202
MAF-6		
	C1	-0.1872
	C2	0.3068
	C3	-0.4654
	C4	-0.6812
	H1	0.1768
	H3	0.2185
	H4	0.2202
	N1	-0.7685
	Zn1	2.6

Figure S2. Schematic representation of the organic linkers of (a) of ZIF-8, (b) ZIF-71, (c) MIL-140C, (d) ZIF-90 and (e) MAF-6. Nitrogen atoms in blue, carbon atoms in cyan, oxygen atoms in red, chlorine in yellow, hydrogen in white and zirconium and zinc atoms in grey. Partial charges of atoms of each MOF. MAF-6 charges have been taken from the literature.[4]

Table S2. Equilibrium adsorption conditions of methanol and ethanol for the selected MOFs.

MOF	Isotherm, Temperature [K]		Isobar, Pressure [kPa]	
	Methanol	Ethanol	Methanol	Ethanol
ZIF-8	298	298	5	0.8
	308	308		
ZIF-71	298	298	8	4
	308	308		
MIL-140C	298	298	1.5	4
ZIF-90	298	298	10	3
	308	308		
MAF-6	298	298	10	2.5

Figure S3 (a) nHB, (b) guest-guest interactions, and (c) host-guest interactions for ethanol as a function of the pressure. Non-depicted error bars denotes fluctuations smaller than symbol size.

Figure S4 f_i (percentage of molecules with n HBs) of (a) methanol and (b) ethanol at 3kPa. (c, d) the same at saturation conditions. Non-depicted error bars denotes fluctuations smaller than symbol size.
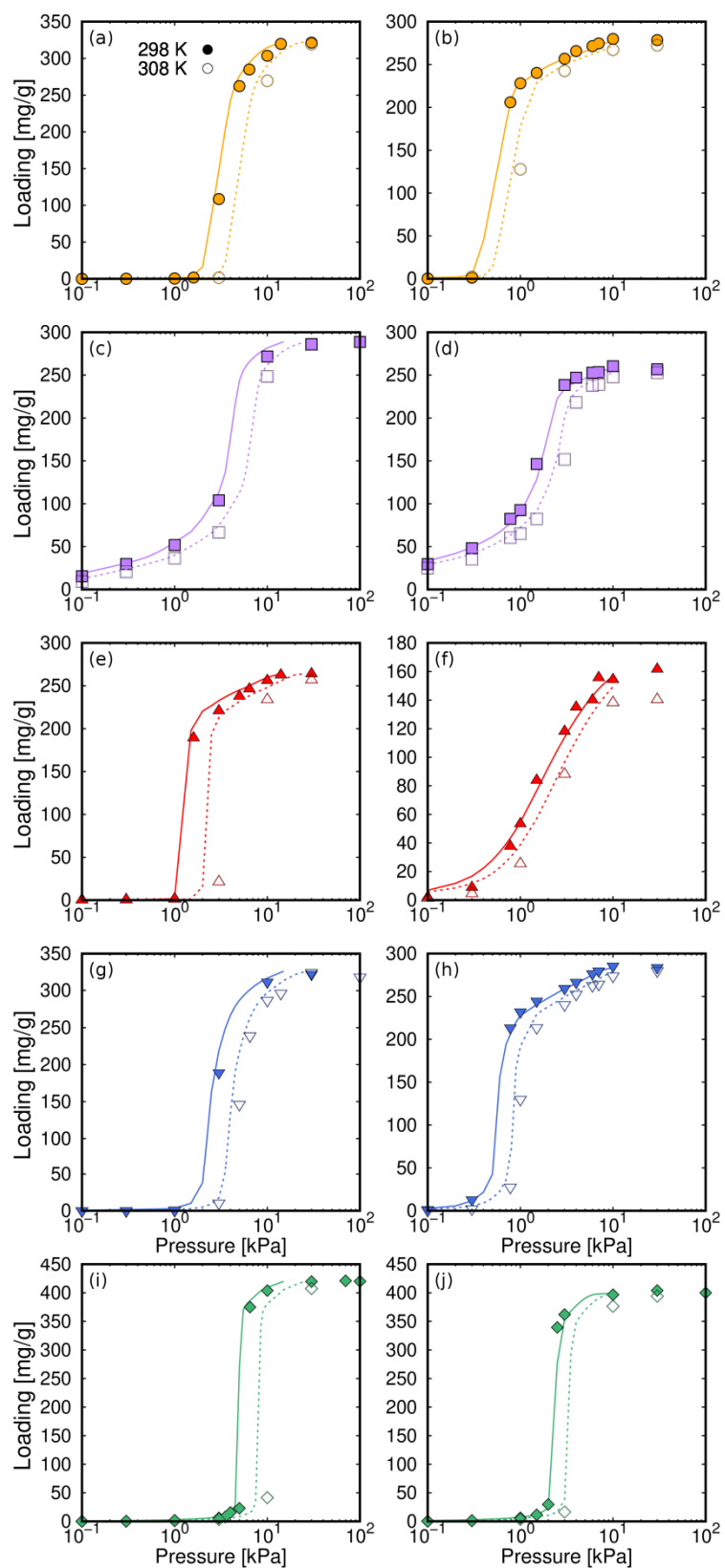
Figure S5 Adsorption isotherms calculated with GCMC simulations (symbols) and from the characteristic curve (lines) of methanol (left column) and ethanol (right column) in (a, b) ZIF-8, (c, d) ZIF-71, (e, f) MIL-140C, (g, h) ZIF-90, and (i, j) MAF-6 at 298 K and 308 K.
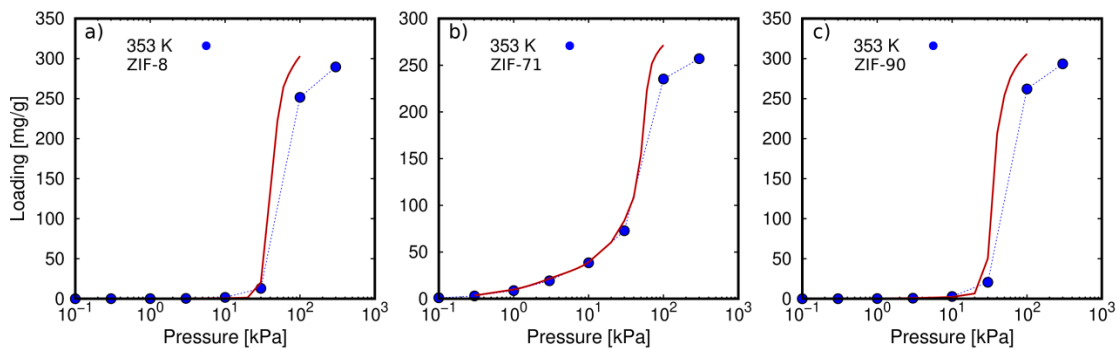
Figure S6. Adsorption isotherms calculated with GCMC simulations (symbols) and from the characteristic curve (lines) of methanol at 353 K in (a) ZIF-8, (b) ZIF-71, and (c) ZIF-90.
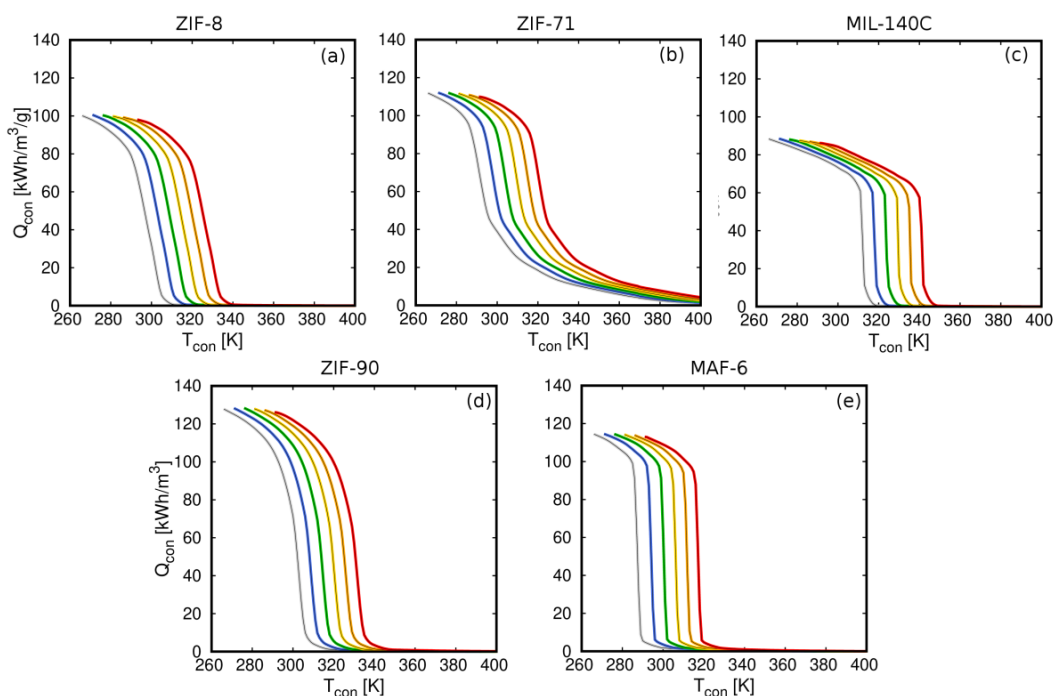

Figure S7. Volumetric heat energy transferred to the condenser (Q_{con}) per unit of volume of MOF using methanol in all MOFs with variation of the temperature of the evaporator assuming full desorption.
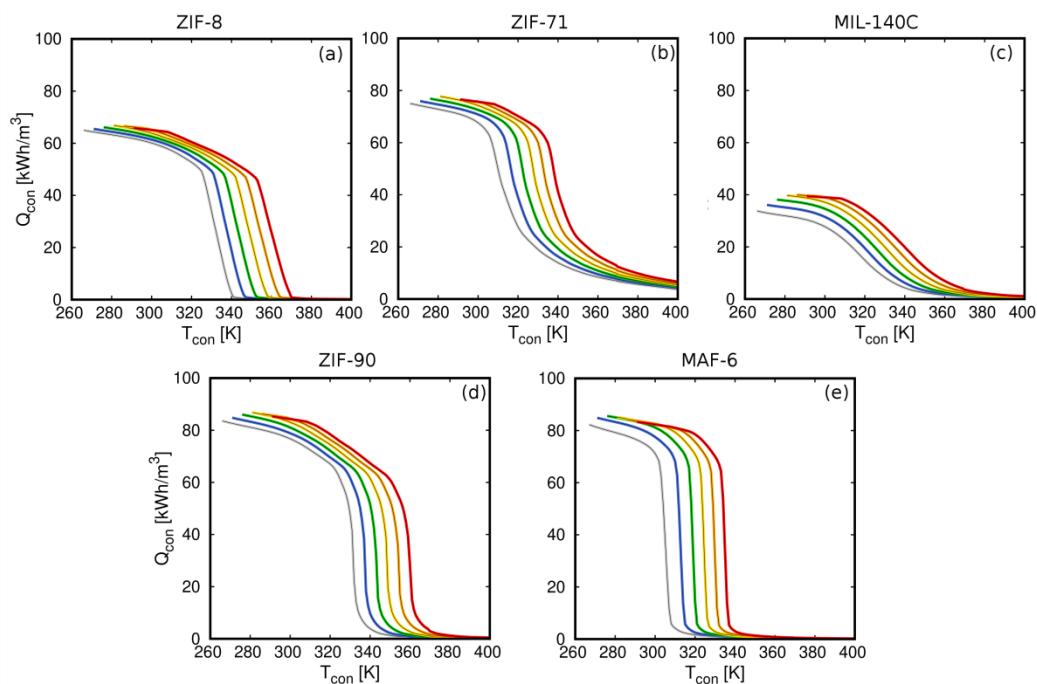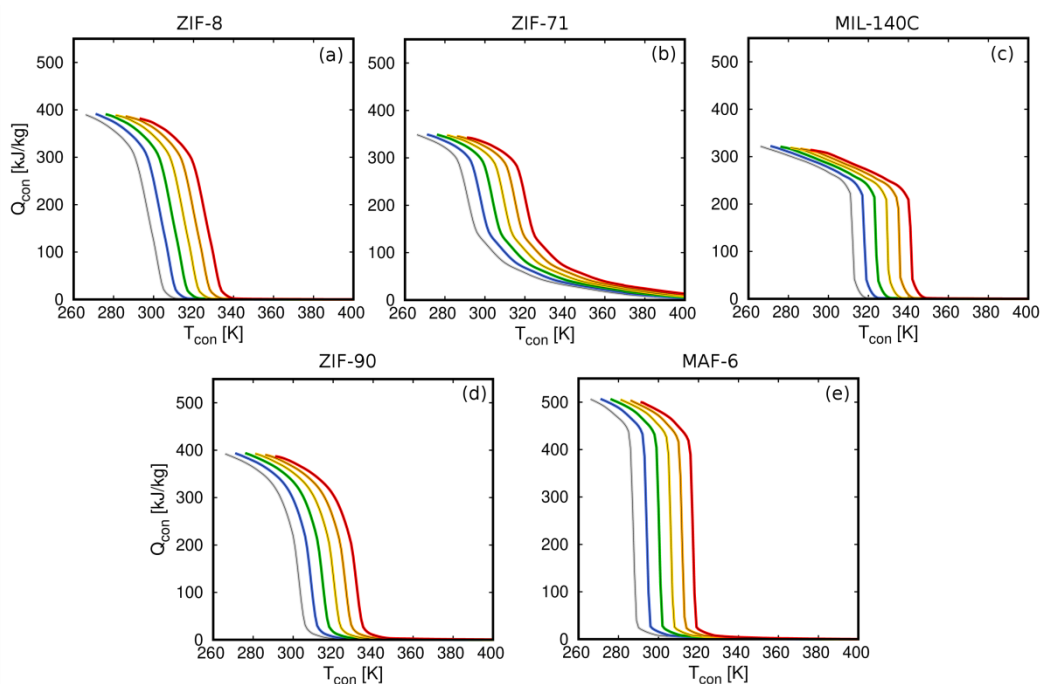
Figure S8. Volumetric heat energy transferred to the condenser (Q_{con}) per unit of volume of MOF using ethanol in all MOFs with variation of the temperature of the evaporator assuming full desorption.

Figure S9. Gravimetric heat energy transferred to the condenser (Q_{con}) per unit of volume of MOF using methanol in all MOFs with variation of the temperature of the evaporator assuming full desorption.
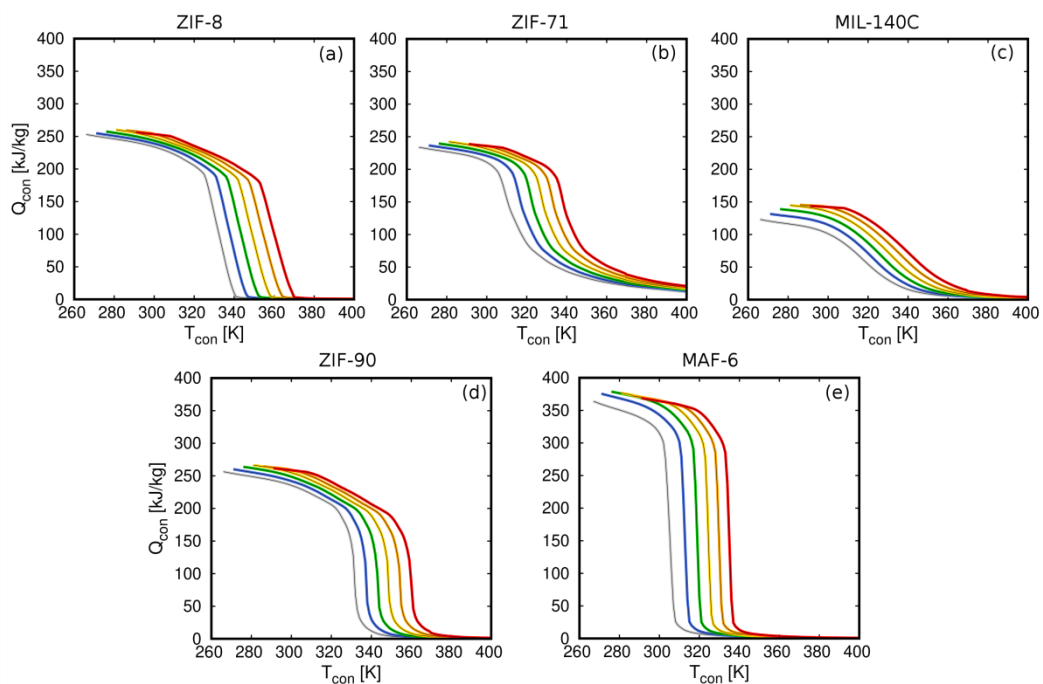
Figure S10. Gravimetric heat energy transferred to the condenser (Q_{con}) per unit of volume of MOF using ethanol in all MOFs with variation of the temperature of the evaporator assuming full desorption.
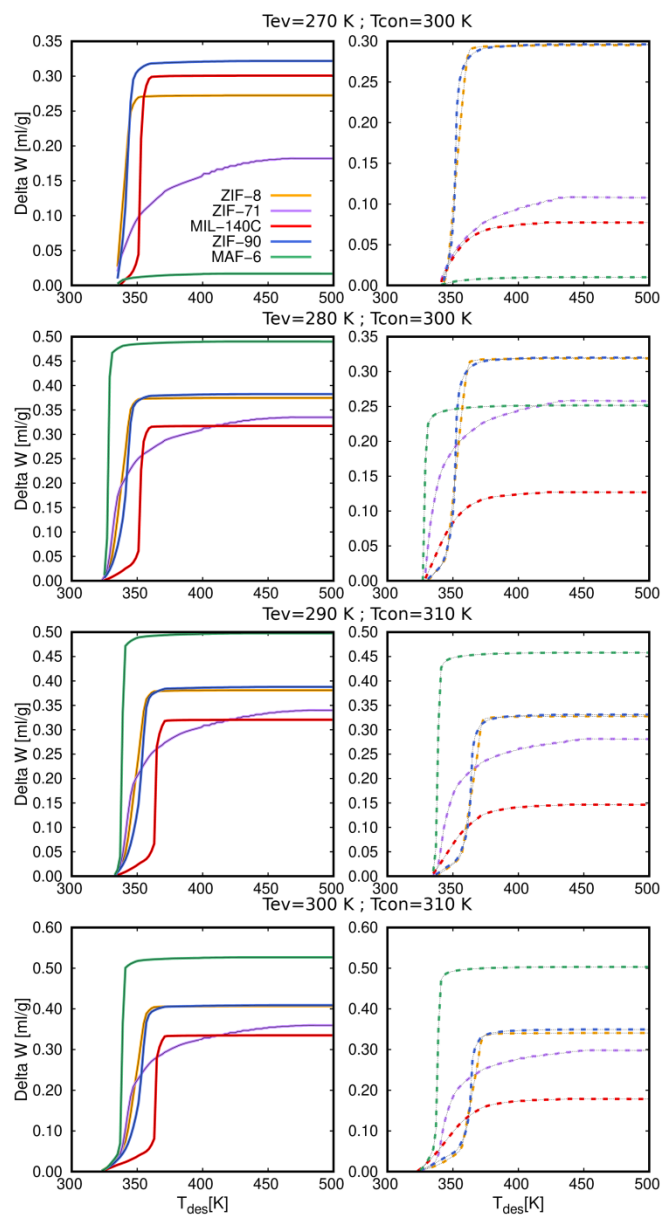
Figure S11. Deliverable capacity for methanol (solid lines) and ethanol (dashed lines) as a function of the desorption temperature for varying the temperatures of the evaporator and condenser.
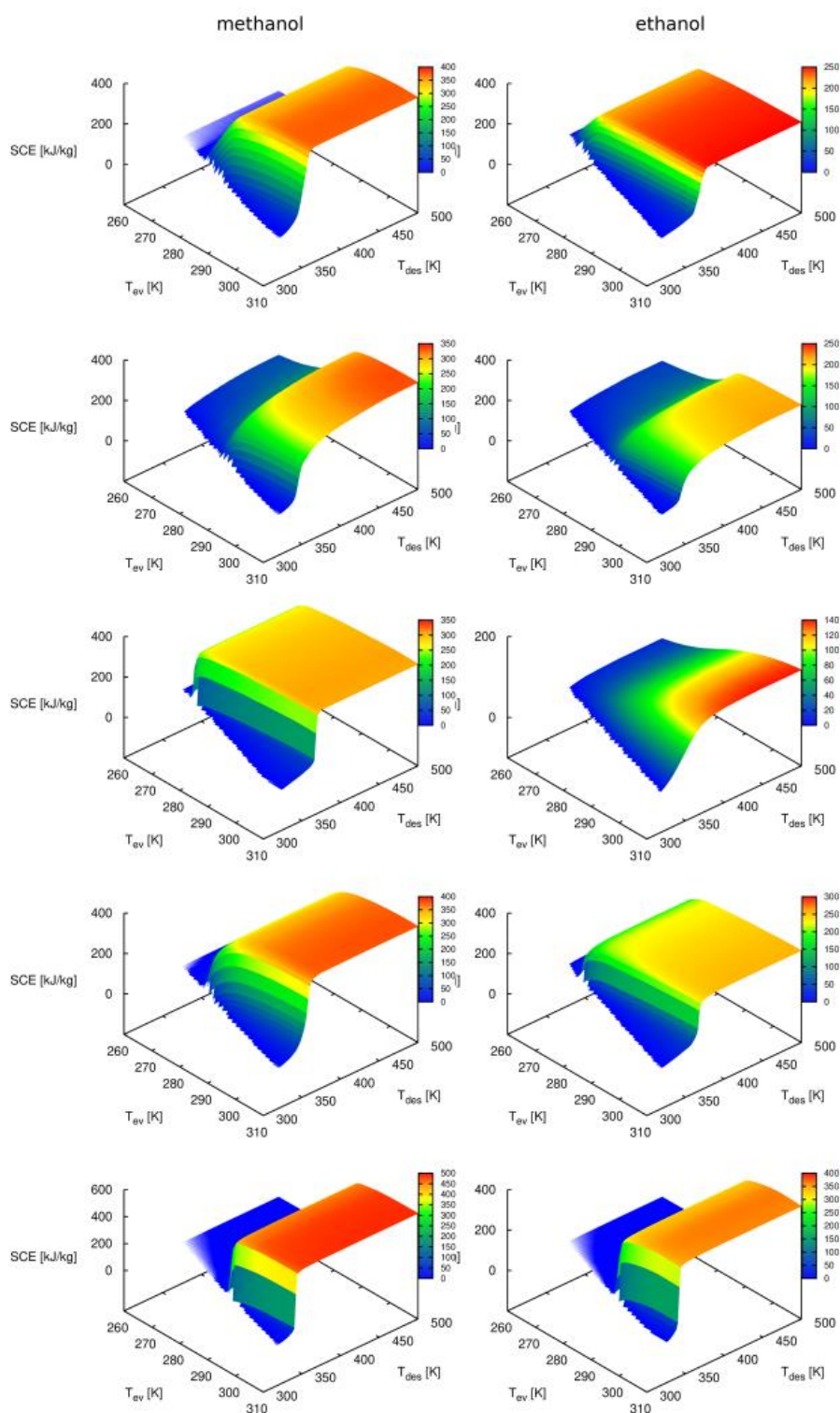
Figure S12. SCE of methanol and ethanol in all MOFs at T_{con}=313 K. From top to bottom, ZIF-8, ZIF-71, MIL-140C, ZIF-90, and MAF-6, respectively.
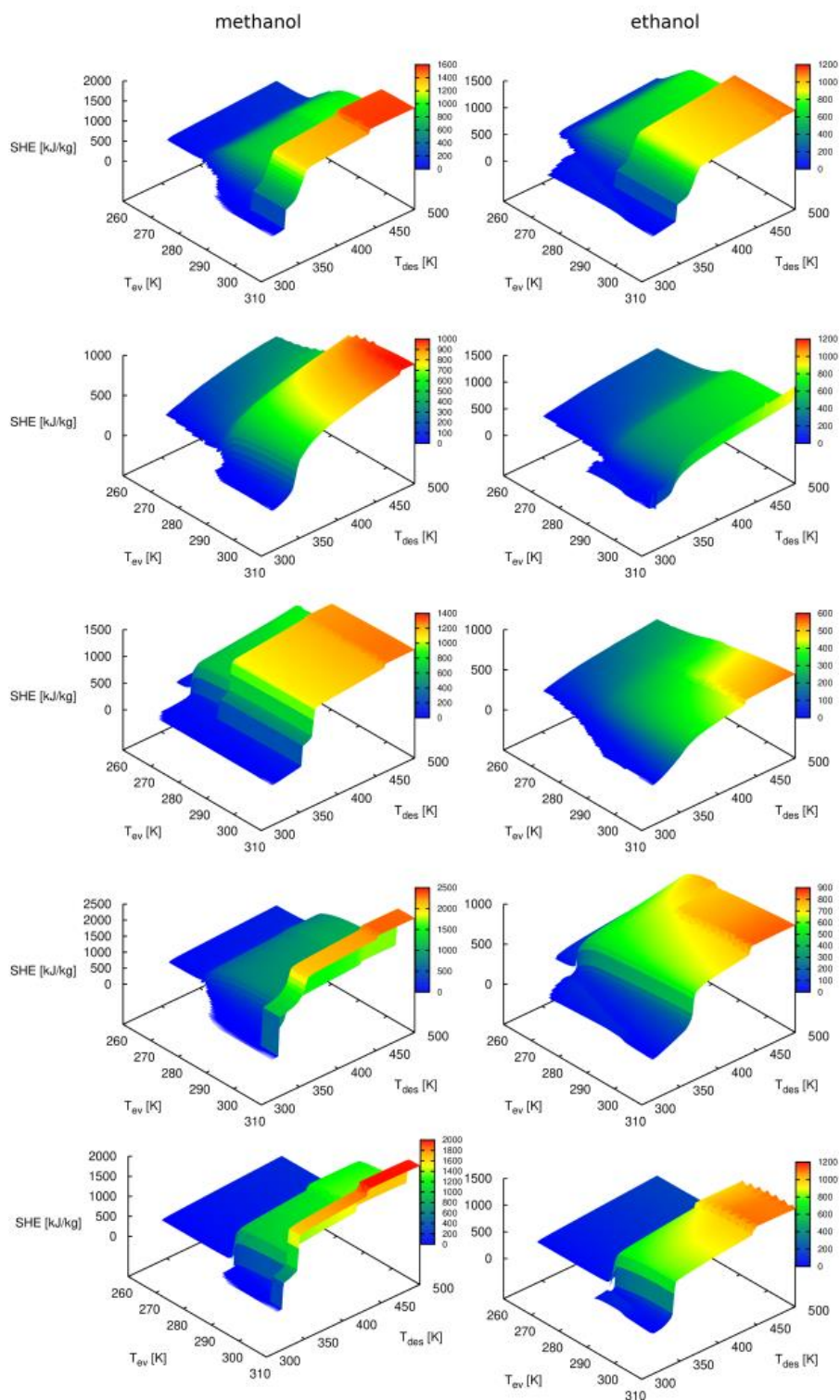
Figure S13. SHE of methanol and ethanol in all MOFs at T_{con}=313 K. From top to bottom, ZIF-8, ZIF-71, MIL-140C, ZIF-90, and MAF-6, respectively.

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