Supplementary Material for: Transport Properties of Mixtures of Acid Gases with Aqueous Monoethanolamine Solutions: A Molecular Dynamics Study

H. Mert Polat[a,b,c], Frédérick de Meyer[a,b], Céline Houriez[b], Christophe Coquelet[b], Othonas A. Moultos[c], Thijs J. H. Vlugt[c,*]

[a] *CCUS and Acid Gas Entity, Liquefied Natural Gas Department, Exploration Production, TotalEnergies S.E., 92078 Paris, France*

[b] *CTP - Centre of Thermodynamics of Processes, Mines ParisTech, PSL University, 35 rue Saint HonorÂĺ, 77305 Fontainebleau, France*

[c] *Engineering Thermodynamics, Process & Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Leeghwaterstraat 39, Delft 2628CB, The Netherlands*

[*] Corresponding author

Email address: t.j.h.vlugt@tudelft.nl (Thijs J. H. Vlugt)

S1. Speedy-Angell Power Equation and Vogel-Tamann-Fulcher Equation

The temperature dependence of values of D_{self} can be described by Speedy-Angell power equation [1] and Vogel-Tamann-Fulcher (VTF) equation [2]. We fit the values of D_{self} of CO_2 and H_2S to Speedy-Angell power equation [1] using:

$$D_{\text{self}} = D_0 \left(\frac{T}{T_s} - 1 \right)^m \tag{S1}$$

where D_0 is the pre-exponential factor, T_s is the singularity temperature and T is the absolute temperature.
We also fit the values of D_{self} of acid gases to VTF equation [2] using:

$$D_{\text{self}} = \exp \left[\frac{-\alpha}{T - \beta} - \gamma \right] \tag{S2}$$

where α, β and γ are the fit parameters.

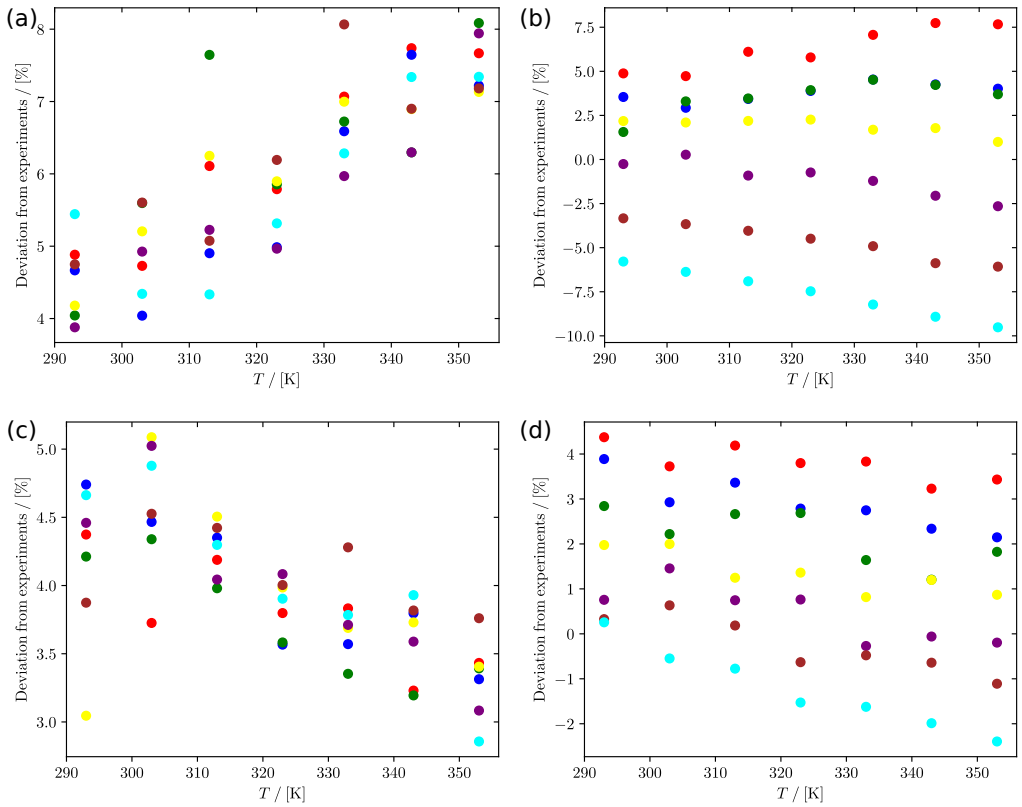

Figure S1: Deviation of the simulated densities of (a,b) pure MEA and (c,d) 30 wt.% MEA/water from experiments [3] as a function of temperature. Subfigures (a) and (c) show the scaling of LJ the ϵ parameters of MEA. Subfigures (b) and (d) show the scaling of the point charges of MEA. The scaling factors are as follows: Red: $\chi = 1.00$; blue: $\chi = 0.95$; green: $\chi = 0.90$; yellow: $\chi = 0.85$; purple: $\chi = 0.80$; brown: $\chi = 0.75$; cyan: $\chi = 0.70$.

Table S1: Force field parameters for monoethanolamine (MEA). For Lennard-Jones (LJ) interactions, the OPLS-AA [4, 5] force field was used while the atomic charges (corresponding to a charge neutral molecule) were computed using quantum chemical calculations. Quantum chemical calculations were performed using Gaussian09 [6] at second order MÃÿller-Plesset perturbation theory (MP2) [7] level using the 6-311+G(2d,2p) basis set. Atomic charges listed in this table are scaled with $\chi = 0.80$.

Atom	ϵ/k_B / [K]	σ / [Å]	q / [e^-]
N_T	85.600	3.30	-0.686816
H_1	1.0000	1.00	0.271816
H_2	1.0000	1.00	0.276432
C_{T1}	33.200	3.50	-0.100352
C_{T2}	33.200	3.50	0.048976
H_{T1}	7.5533	2.50	0.108248
H_{T2}	7.5533	2.50	0.133688
H_{T3}	15.107	2.50	0.099312
H_{T4}	15.107	2.50	0.106488
O_H	85.605	3.12	-0.628376
H_O	1.0000	1.00	0.370584

Table S2: Force field parameters for carbon dioxide. The TraPPE [8] force field was used for carbon dioxide.

Atom	ϵ/k_{B} / [K]	σ / [Å]	q / $[e^{-}]$
O	79.0	3.05	-0.35
C	27.0	2.80	0.70

Table S3: Force field parameters for hydrogen sulfide. The force field from KristÃşf and Lizsi [9] was used. X corresponds to the dummy charge site in force field developed by KristÃşf and Lizsi.

Atom	ϵ/k_{B} / [K]	σ / [Å]	q / [e^{-}]
S	250.0	3.73	0.40
H	1.000	1.00	0.25
X	1.000	1.00	-0.90

Table S4: Computed viscosities of pure MEA and 30 wt.% MEA solutions. The subscripts in the second and third column show uncertainties computed as one standard deviation.

Temperature / [K]	Viscosity / [cP]	
	Pure MEA	30 wt.% MEA/water
293	$26.26_{2.2}$	$2.69_{0.1}$
298	$20.05_{1.6}$	$2.35_{0.1}$
303	$16.14_{1.2}$	$2.13_{0.1}$
308	$12.95_{1.1}$	$1.97_{0.2}$
313	$10.70_{1.6}$	$1.68_{0.2}$
323	$7.22_{0.6}$	$1.39_{0.1}$
333	$4.72_{0.4}$	$1.20_{0.1}$
343	$3.20_{0.6}$	$0.99_{0.1}$
353	$2.42_{0.2}$	$0.91_{0.1}$

Table S5: Computed self-diffusivities of MEA and water in pure MEA and 30 wt.% MEA solutions. The subscripts in the second, third, and fourth column show uncertainties computed as one standard deviation.

Temperature / [K]	D_{self} / $10^{-11} \times [\text{m}^2\,\text{s}^{-1}]$		
	Pure MEA	30 wt.% MEA/water	
	MEA	MEA	Water
293	$4.32_{0.7}$	$31.22_{2.4}$	$72.42_{4.0}$
298	$5.62_{1.0}$	$35.22_{5.3}$	$82.53_{4.0}$
303	$9.87_{2.3}$	$41.07_{2.0}$	$93.64_{5.6}$
308	$11.00_{1.9}$	$43.47_{3.9}$	$98.46_{3.5}$
313	$13.67_{2.2}$	$53.45_{4.3}$	$118.99_{5.6}$
323	$21.21_{1.2}$	$64.20_{3.3}$	$145.54_{6.2}$
333	$30.83_{1.8}$	$74.68_{2.6}$	$172.67_{7.0}$
343	$46.41_{2.2}$	$96.20_{7.9}$	$206.14_{12.3}$
353	$61.64_{2.4}$	$118.50_{3.8}$	$256.67_{5.4}$

Table S6: Computed self-diffusion coefficients of CO_2 as a function of temperature and MEA concentration in the solution. The subscripts show uncertainties computed as one standard deviation.

Temperature / [K]	D_{self} / $10^{-10} \times [\text{m}^2\,\text{s}^{-1}]$				
	10 wt.% MEA/water	20 wt.% MEA/water	30 wt.% MEA/water	40 wt.% MEA/water	50 wt.% MEA/water
293	$21.27_{0.6}$	$18.58_{1.3}$	$10.68_{1.2}$	$5.71_{0.4}$	$2.82_{0.4}$
298	$22.76_{2.1}$	$22.17_{2.0}$	$13.84_{1.3}$	$6.91_{0.7}$	$4.12_{0.2}$
303	$23.67_{1.8}$	$25.46_{1.8}$	$14.18_{2.0}$	$7.70_{1.0}$	$4.25_{0.7}$
308	$26.94_{2.9}$	$26.15_{2.0}$	$16.99_{1.9}$	$9.39_{1.2}$	$5.32_{0.4}$
313	$31.13_{2.0}$	$30.69_{2.3}$	$20.90_{3.5}$	$12.37_{1.3}$	$7.71_{0.5}$
323	$36.29_{2.4}$	$34.44_{2.4}$	$19.66_{2.3}$	$13.54_{0.9}$	$8.47_{0.3}$
333	$39.25_{2.1}$	$38.07_{2.3}$	$25.97_{0.8}$	$14.43_{1.6}$	$10.02_{1.8}$
343	$46.42_{3.0}$	$43.29_{3.5}$	$29.51_{6.2}$	$17.91_{1.5}$	$10.36_{1.7}$
353	$50.95_{2.3}$	$50.83_{2.9}$	$35.30_{4.3}$	$19.06_{2.5}$	$14.11_{2.2}$

Table S7: Computed self-diffusion coefficients of H_2S as a function of temperature and MEA concentration in the solution. The subscripts show uncertainties computed as one standard deviation.

Temperature / [K]	D_{self} / $10^{-10} \times [\text{m}^2\,\text{s}^{-1}]$				
	10 wt.% MEA/water	20 wt.% MEA/water	30 wt.% MEA/water	40 wt.% MEA/water	50 wt.% MEA/water
293	$16.32_{1.5}$	$12.86_{1.4}$	$9.29_{0.8}$	$4.29_{0.4}$	$2.40_{0.2}$
298	$16.10_{1.4}$	$12.95_{1.1}$	$10.09_{0.8}$	$4.97_{0.3}$	$3.26_{0.3}$
303	$17.14_{1.5}$	$15.40_{0.7}$	$11.24_{0.6}$	$6.31_{0.4}$	$3.69_{0.3}$
308	$21.21_{1.3}$	$16.37_{2.5}$	$14.05_{1.2}$	$6.45_{0.5}$	$4.15_{0.3}$
313	$25.13_{3.0}$	$18.78_{2.0}$	$15.58_{1.4}$	$8.26_{0.8}$	$4.83_{0.5}$
323	$28.03_{2.4}$	$23.18_{2.1}$	$19.43_{1.4}$	$10.02_{0.5}$	$6.19_{0.3}$
333	$31.38_{2.7}$	$27.20_{2.9}$	$22.57_{2.2}$	$12.25_{1.8}$	$9.22_{0.7}$
343	$37.91_{2.3}$	$33.33_{2.6}$	$27.00_{3.9}$	$15.02_{0.9}$	$10.61_{0.8}$
353	$45.48_{3.5}$	$34.88_{1.4}$	$30.63_{3.2}$	$20.32_{1.2}$	$13.23_{0.5}$

Table S8: Speedy-Angell power equation [1] ($D_{\text{self}} = D_0 \left(\frac{T}{T_s} - 1\right)^m$) fit parameters ($D_0$, T_{S} and m) and coefficient of determinations (R^2) for D_{self} of CO_2 in MEA/water solutions for different MEA concentrations. The values of D_{self} of CO_2 were fitted for a temperature range of 293–353 K.

MEA concentration / [wt.%]	D_0 / [$m^2\,s^{-1}$]	T_{S} / [K]	m	R^2
10	1.27×10^{-8}	238.84	1.23	0.991
20	1.25×10^{-8}	241.44	1.19	0.990
30	8.63×10^{-9}	220.23	1.80	0.971
40	4.80×10^{-9}	282.68	0.65	0.978
50	4.33×10^{-9}	280.31	0.87	0.961

Table S9: Speedy-Angell power equation [1] ($D_{\text{self}} = D_0 \left(\frac{T}{T_s} - 1\right)^m$) fit parameters ($D_0$, T_{S} and m) and coefficient of determinations (R^2) for D_{self} of H_2S in MEA/water solutions for different MEA concentrations. The values of D_{self} of H_2S were fitted for a temperature range of 293–353 K.

MEA concentration / [wt.%]	D_0 / [$m^2\,s^{-1}$]	T_{S} / [K]	m	R^2
10	4.31×10^{-10}	120.58	3.57	0.985
20	1.11×10^{-8}	245.76	1.36	0.988
30	1.08×10^{-8}	258.05	1.26	0.997
40	3.63×10^{-35}	0.2031	7.94	0.992
50	6.78×10^{-9}	234.98	2.37	0.993

Table S10: Vogel-Tamann-Fulcher (VTF) equation [2] ($D_{\text{self}} = \exp\left[\frac{-\alpha}{T-\beta} - \gamma\right]$) fit parameters ($\alpha$, β, γ) and coefficient of determinations (R^2) for D_{self} of CO_2 in MEA/water solutions for different MEA concentrations. The values of D_{self} of CO_2 were fitted for a temperature range of 293–353 K.

MEA concentration / [wt.%]	α	β	γ	R^2
10	385.62	161.30	17.08	0.992
20	432.29	151.94	16.97	0.990
30	861.74	101.79	16.04	0.971
40	78.726	254.40	19.28	0.979
50	133.60	243.50	19.22	0.960

Table S11: Vogel-Tamann-Fulcher (VTF) equation [2] ($D_{\text{self}} = \exp\left[\frac{-\alpha}{T-\beta} - \gamma\right]$) fit parameters ($\alpha$, β, γ) and coefficient of determinations (R^2) for D_{self} of H_2S in MEA/water solutions for different MEA concentrations. The values of D_{self} of H_2S were fitted a the temperature range of 293–353 K.

MEA concentration / [wt.%]	α	β	γ	R^2
10	3069.55	-93.855	12.35	0.985
20	367.787	179.11	17.33	0.989
30	300.548	199.11	17.65	0.997
40	208598	-2604.8	-50.49	0.992
50	804.827	150.63	16.46	0.993

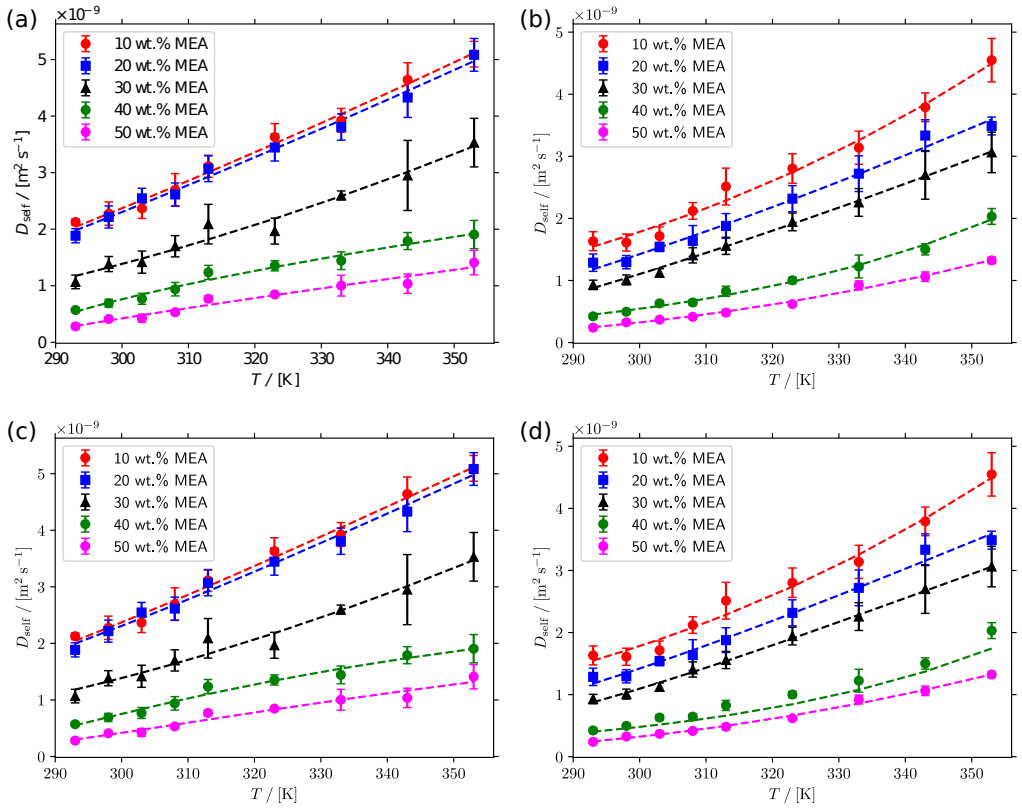

Figure S2: Computed values of D_{self} of (a,c) CO_2 and (b,d) H_2S as a function of temperature and MEA concentration in the solution. The dashed lines represent the fits to (a,b) Speedy-Angell power equation [1] and (c,d) Vogel-Tamann-Fulcher equation [2].

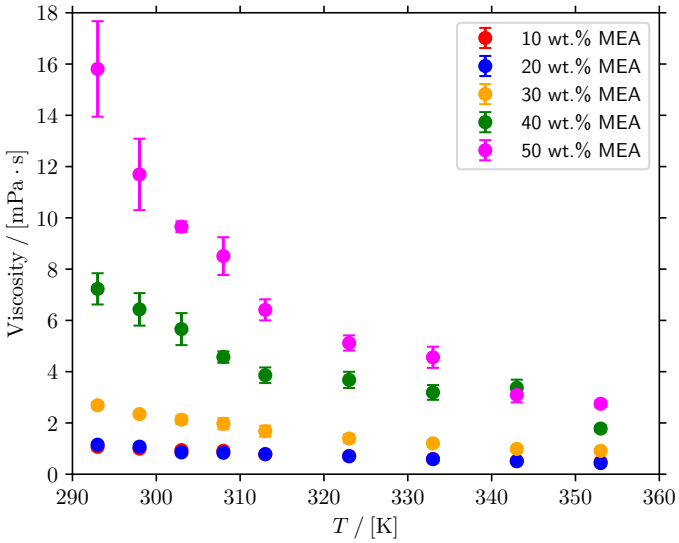

Figure S3: Computed viscosities of MEA/water solutions as a function of temperature and MEA concentration in the solution.

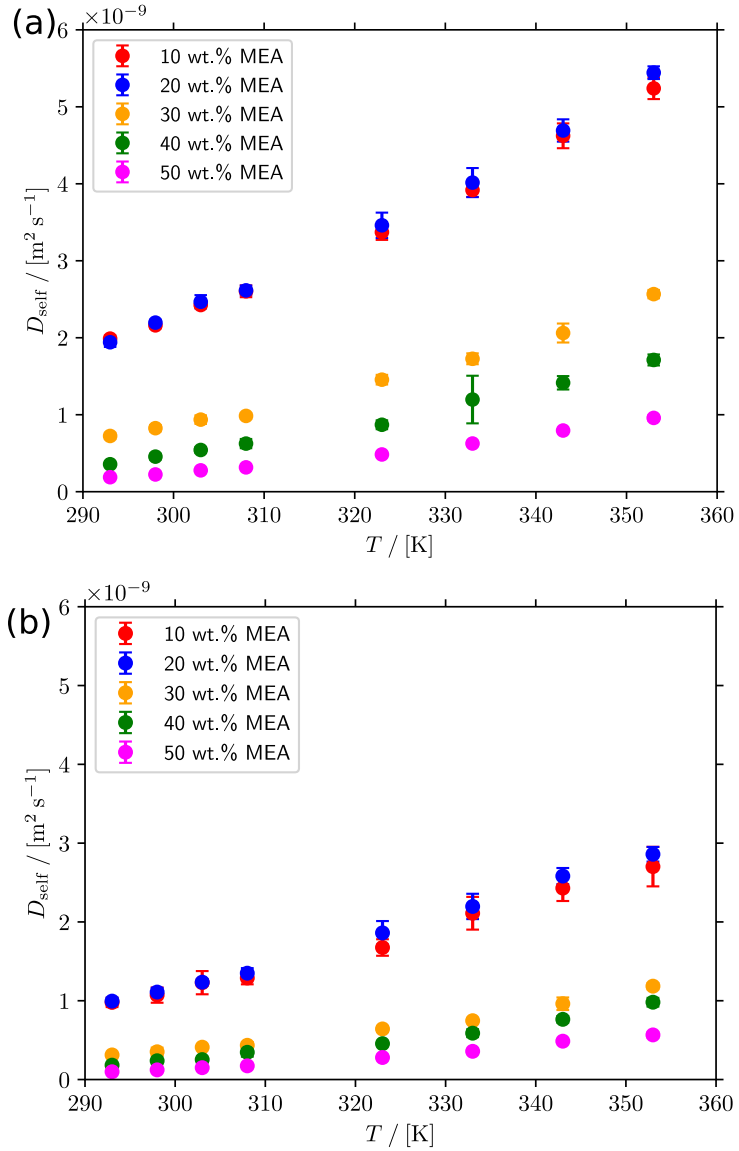

Figure S4: Computed values of D_{self} of (a) water and (b) MEA molecules as a function of temperature and MEA concentration in the solution.

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