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Supplementary materials

Diffusion Coefficients in Systems Related to Reservoir Fluids: Available Data and Evaluation of Correlations

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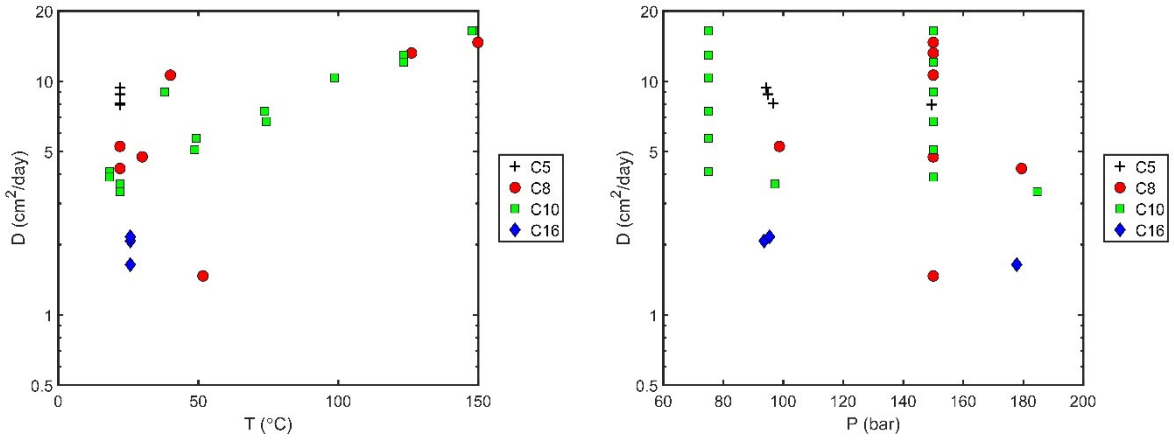
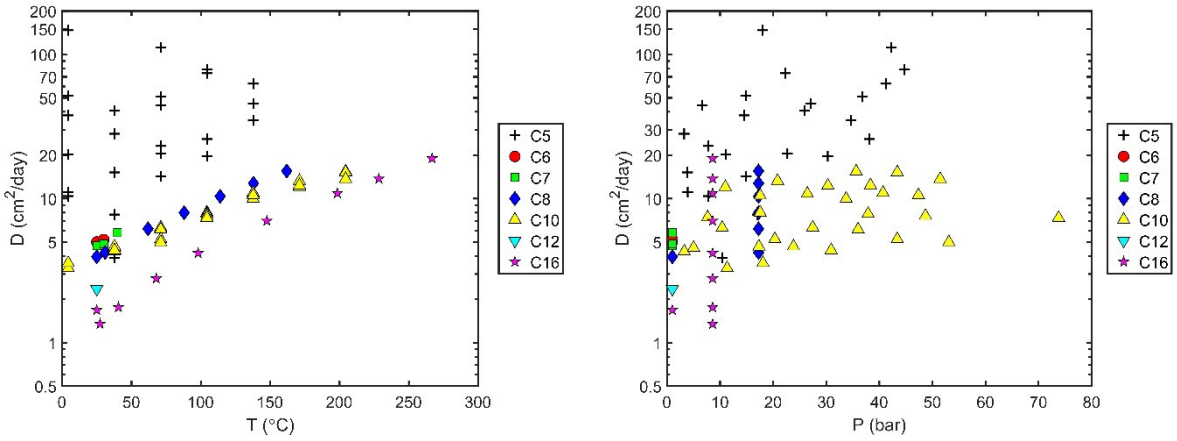
We provide some supplementary figures to the manuscript. Figures S1-S4 are about the data trends in N_2-C_n, C_2-C_n, C_3-C_n, C_4-C_n, and C_{10}/C_{12}/C_{14}/C_{16}/-C_n. Figures S5-S8 are the results including the C_1-C_{10} data from Dysthe et al. (1995). They correspond to Figures 10, 11, 12, and 16 in the manuscript.

In addition, we provide Table S1 that provides the detailed AAD% for different binary mixtures using various correlations. Table S1 corresponds to the base case calculation discussed in "Whole concentration range" in Section 5.2.



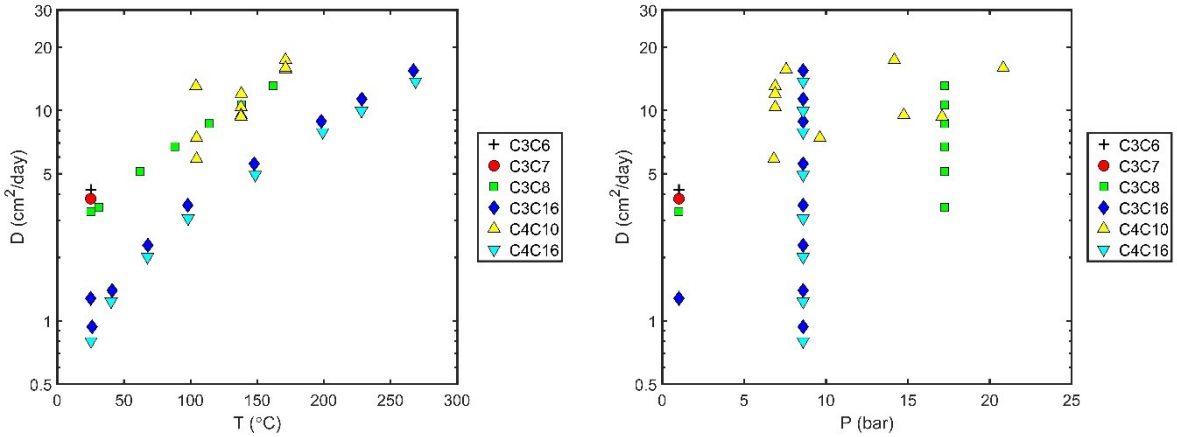
(**a**) (**b**)

Figure S1. Liquid-phase diffusion coefficients for N_2-C_n systems: (**a**) Temperature dependence; (**b**) Pressure dependence.



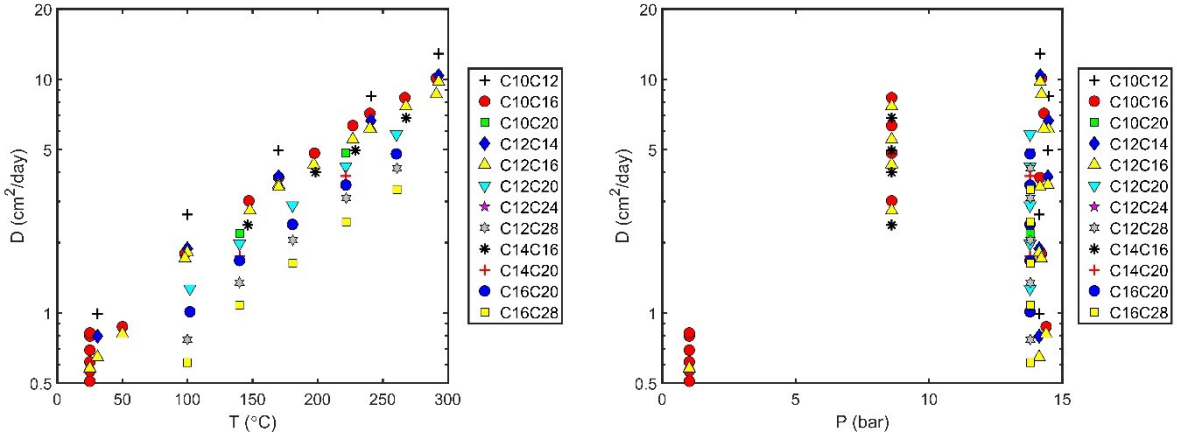
(**a**) (**b**)

Figure S2. Liquid-phase diffusion coefficients for C_2-C_n systems: (**a**) Temperature dependence; (**b**) Pressure dependence.



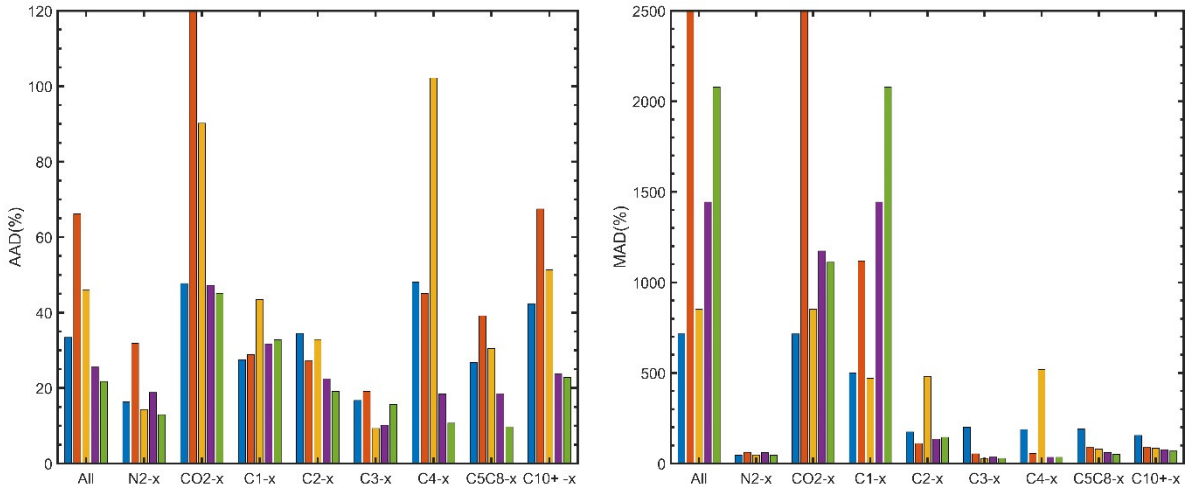
(**a**) (**b**)

Figure S3. Liquid-phase diffusion coefficients for C_3/C_4-C_n systems: (**a**) Temperature dependence; (**b**) Pressure dependence.



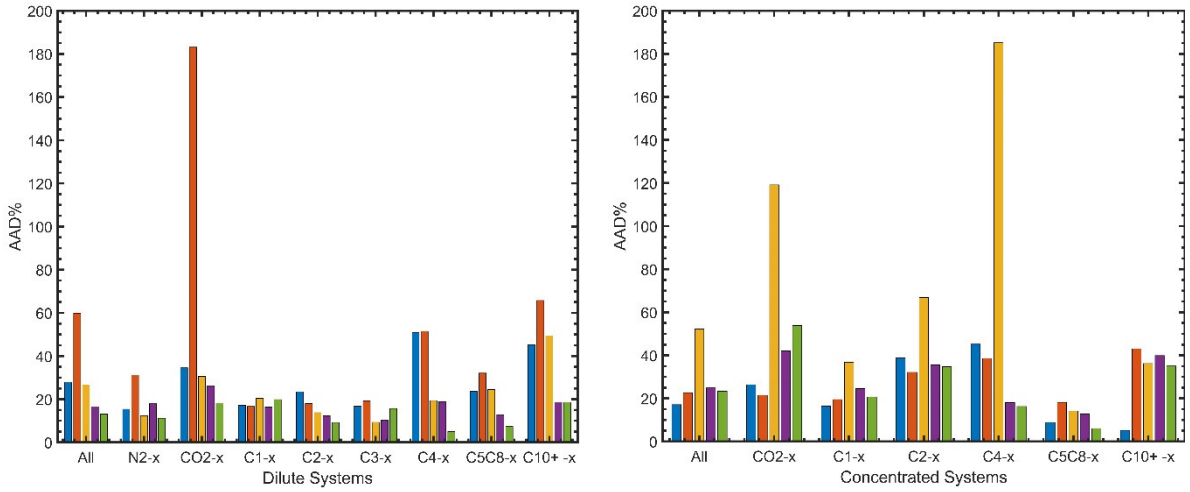
(**a**) (**b**)

Figure S4. Liquid-phase diffusion coefficients for C_{10}/C_{12}/C_{14}/C_{16}-C_n systems: (**a**) Temperature dependence; (**b**) Pressure dependence.



(**a**) (**b**)

Figure S5. Deviations for the base case calculation using different correlations: (**a**) AAD%; (**b**) MAD% (blue for ES; red for RW; yellow for LF; purple for WC; green for HM). Corresponding to Figure 10.



(**a**) (**b**)

Figure S6. Deviations for the base case: (**a**) dilute concentration range; (**b**) concentrated systems (blue for ES; red for RW; yellow for LF; purple for WC; green for HM). Corresponding to Figure 11.

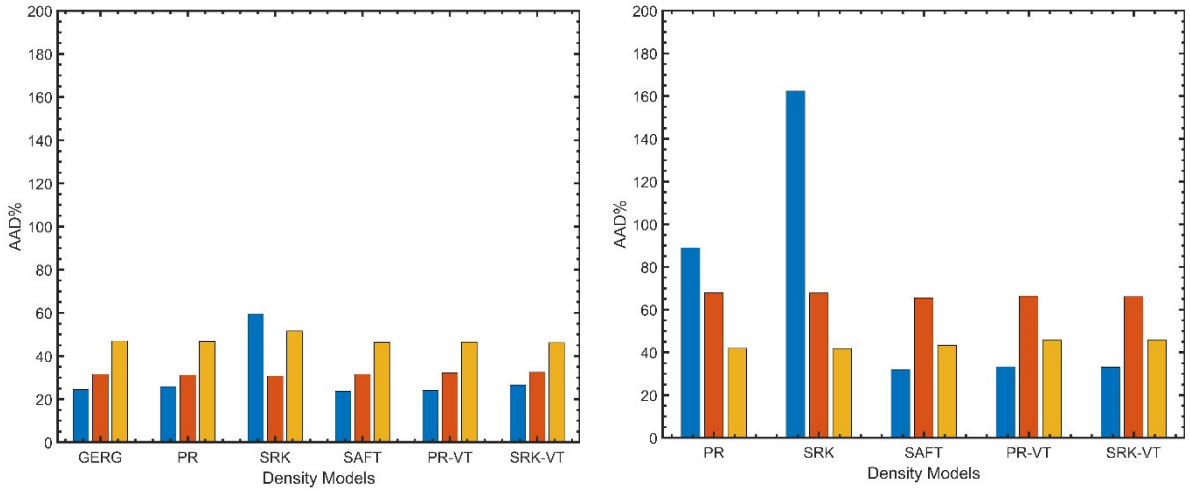


Figure S7. Deviations for (**a**) 32 "GERG systems" and (**b**) all 72 systems with different density models (blue for ES; red for RW; yellow for LF). Corresponding to Figure 12.

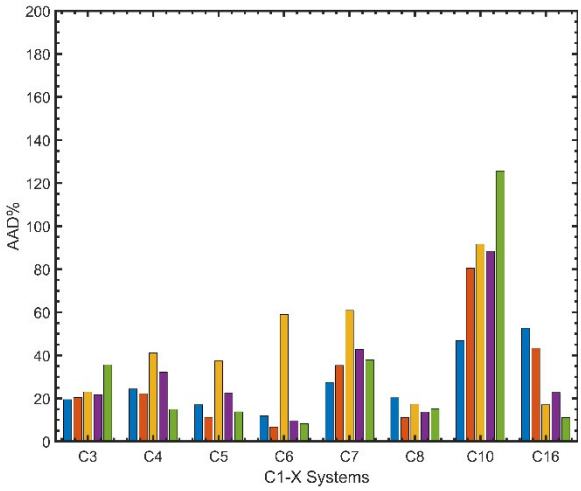


Figure S8. Deviations for C_1-X systems with default settings. Corresponding to Figure 16(a).

Table S1. AAD% in diffusion coefficients calculated by different correlations (base case calculation).

System	Np*	ES	RW	LDF	WC	HM
N_2-C_8	5	12.3	29.6	12.9	15.7	10.8
N_2-C_{10}	12	18.5	32.8	11.9	20.0	11.6
CO_2-C_5	14	31.9	64.9	250.6	109.6	96.5
CO_2-C_6	21	25.2	56.2	13.2	17.9	12.4
CO_2-C_7	85	76.1	66.3	70.3	85.2	80.4
CO_2-C_8	45	25.7	48.6	57.5	26.1	26.0
CO_2-C_9	5	56.3	63.3	49.5	37.5	30.7
CO_2-C_{10}	36	35.9	39.2	107.7	37.5	43.2
CO_2-C_{11}	5	54.1	64.2	48.3	42.0	35.6
CO_2-C_{12}	29	27.9	51.1	31.3	29.2	11.2

CO_2-C_{14}	29	55.8	38.5	251.8	77.2	140.9
CO_2-C_{16}	73	55.4	1668.8	68.0	49.0	39.2
CO_2-C_{20}	5	48.6	75.6	55.5	19.8	7.0
CO_2-C_{28}	5	79.9	89.4	78.5	35.7	18.6
C_1-C_3	22	19.5	20.4	23.0	21.7	35.7
C_1-C_4	19	24.4	22.2	41.1	32.2	14.9
C_1-C_5	42	17.0	11.2	37.4	22.4	13.8
C_1-C_6	1	11.9	6.7	59.1	9.7	8.3
C_1-C_7	56	27.4	35.3	60.9	42.9	37.9
C_1-C_8	12	20.3	11.1	17.3	13.7	15.2
C_1-C_{10}	49	30.3	47.7	103.1	39.2	48.4
C_1-C_{16}	8	52.6	43.3	17.1	22.8	11.1
C_2-C_5	26	65.5	64.5	79.2	60.2	61.5
C_2-C_6	2	18.7	15.8	23.5	10.2	23.3
C_2 -C_7	3	6.4	3.1	12.9	2.9	10.5
C_2-C_8	7	7.5	14.4	10.1	6.2	4.5
C_2-C_{10}	30	27.2	19.7	74.5	29.3	23.0
C_2-C_{12}	1	59.1	25.6	17.2	25.4	6.7
C_2-C_{16}	9	57.0	47.1	12.6	23.0	4.3
C_3-C_6	1	5.7	6.9	5.6	11.4	28.6
C_3-C_7	1	0.8	1.0	8.3	3.5	21.1
C_3-C_8	7	5.3	20.9	7.0	5.2	7.5
C_3-C_{16}	9	55.0	47.8	16.3	20.6	5.5
C_4-C_{10}	8	45.2	38.6	185.1	18.1	16.3
C_4-C_{16}	8	50.9	51.5	19.3	18.7	5.1
C_5-C_6	1	19.4	23.2	29.3	15.5	1.2
C_5-C_8	6	14.7	33.1	9.2	6.6	1.8
C_5-C_{16}	8	51.8	53.2	22.9	16.9	6.0
C_6-C_7	40	18.8	25.3	28.4	12.3	2.6
C_6-C_8	31	16.9	25.2	26.0	11.9	5.4
C_6-C_{10}	1	24.5	28.0	33.4	15.0	3.0
C_6-C_{12}	39	27.6	32.0	26.6	21.2	8.6
C_6-C_{16}	11	47.0	40.0	31.9	33.7	18.6
C_6-C_{18}	1	22.3	29.7	34.1	10.0	1.4
C_6-C_{24}	1	23.4	30.4	32.5	12.4	4.9
C_6-C_{32}	1	30.4	38.6	35.8	27.5	20.5
C_7-C_8	45	15.3	28.9	23.4	9.6	3.3
C_7-C_{10}	26	17.1	32.6	26.5	18.9	7.5
C_7-C_{12}	33	18.8	31.4	22.1	16.8	9.9
C_7-C_{14}	29	30.8	36.1	24.9	25.6	13.0
C_7-C_{16}	18	31.1	40.8	25.0	18.7	10.5
C_7-C_{18}	1	3.6	48.8	31.7	32.5	6.0
C_8-C_{10}	6	24.0	40.5	14.1	9.4	4.3
C_8-C_{12}	36	19.1	37.8	23.0	14.8	7.3
C_8-C_{14}	30	30.5	37.4	24.5	22.9	11.2
C_8-C_{16}	16	35.7	54.1	34.6	15.9	7.9

C_8-C_{20}	5	42.6	73.0	53.0	18.1	21.3
C_8-C_{24}	1	13.7	34.7	34.5	19.6	13.3
C_8-C_{28}	5	74.5	86.9	76.6	35.8	36.9
C_8-C_{32}	1	15.1	37.5	37.5	21.2	16.9
C_{10}-C_{12}	5	26.4	47.9	24.0	16.7	7.7
C_{10}-C_{16}	20	56.6	49.2	32.2	17.4	7.6
C_{10}-C_{20}	2	45.0	73.3	54.6	17.3	22.3
C_{12}-C_{14}	5	25.4	48.1	24.8	16.8	6.2
C_{12}-C_{16}	16	40.2	54.3	34.0	14.9	8.5
C_{12}-C_{20}	5	43.4	73.5	56.9	17.4	23.8
C_{12}-C_{24}	1	0.4	79.8	68.1	75.9	68.7
C_{12}-C_{28}	5	74.1	86.7	79.3	33.7	38.1
C_{14}-C_{16}	9	31.3	61.5	41.9	14.2	9.3
C_{14}-C_{20}	2	46.5	74.0	58.4	14.9	22.5
C_{16}-C_{20}	5	44.8	74.3	60.5	15.8	23.4
C_{16}-C_{28}	5	73.9	86.6	81.4	29.3	36.1
Summary						
All	1162	33.2	65.7	46.0	24.8	20.6
N_2-X	17	15.4	31.2	12.4	17.9	11.2
CO_2-X	352	47.7	193.8	90.2	47.2	45.1
C_1-X	209	25.4	24.7	44.9	25.6	23.1
C_2-X	78	34.5	27.2	32.9	22.5	19.1
C_3-X	18	16.7	19.1	9.3	10.2	15.7
C_4-X	16	48.1	45.1	102.2	18.4	10.7
C_5-C_8 -X	392	26.7	39.1	30.5	18.5	9.7
C_{10+} -X	80	42.3	67.4	51.3	23.7	22.8

* Np is the number of the liquid-phase diffusion coefficients with the composition information.

Reference

Dysthe, D.; Hafskjold, B. Inter-and Intradiffusion in Liquid Mixtures of Methane and n-Decane. *International journal of thermophysics* **1995**, *16*, 1213–1224.