Molecular Simulation and Macroscopic Modeling of the Diffusion of Hydrogen, Carbon Monoxide and Water in Heavy n-Alkane Mixtures

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Supplementary Material

January 2012

Table S1. Experimental values and MD predictions at 3.4 MPa for the melt density of the *n*-alkane mixtures. The "experimental" density of *n*-alkane mixtures was obtained from linear correlation of the experimental density values of the pure *n*-alkanes.

T (K)	Density (g/cm^3)		
	"Experimental"	**Simulation**	**% Abs Dev**
		Mixture A	
473	0.733	0.744 ± 0.002	1.5
493	0.719	0.732 ± 0.001	1.8
513	0.709	0.718 ± 0.002	1.3
		Mixture B	
473	0.722	0.733 ± 0.001	1.5
493	0.707	0.721 ± 0.001	2.0
513	0.696	0.708 ± 0.001	1.7
		Mixture C	
473	0.692	0.704 ± 0.002	1.7
493	0.677	0.690 ± 0.001	1.9
513	0.663	0.679 ± 0.001	2.4
		Mixture D	
473	0.668	0.680 ± 0.001	1.8
493	0.652	0.665 ± 0.001	2.0
513	0.637	0.651 ± 0.001	2.2
		Mixture E	
473	0.719	0.729 ± 0.001	1.4
493	0.704	0.718 ± 0.001	2.0
513	0.693	0.705 ± 0.001	1.7
		Mixture F	
473	0.688	0.702 ± 0.001	2.0
493	0.672	0.688 ± 0.001	2.4
513	0.659	0.674 ± 0.001	2.3
		Mixture G	
473	0.692	0.697 ± 0.001	0.7
493	0.675	0.689 ± 0.001	2.1
513	0.661	0.676 ± 0.002	2.3
		Mixture H	
473	0.692	0.703 ± 0.002	1.6
493	0.675	0.692 ± 0.001	2.5
513	0.663	0.675 ± 0.006	1.8

Table S2. Re-adjusted values of constants β and V_D in eq. (4) for H_2, CO and H_2O in various *n*-alkanes.

	H_2	CO	H_2O	
Solvent		**β**		**V_D**
***n*-C_8**	0.0278	0.0187	0.0213	136.8
***n*-C_{12}**	0.0268	0.0141	0.0172	203.4
***n*-C_{16}**	0.0213	0.0104	0.0133	265.2
***n*-C_{20}**	0.0194	0.0102	0.0131	344.4
***n*-C_{28}**	0.0131	0.0060	0.0078	447.7
***n*-C_{64}**	0.0066	0.0025	0.0036	1034.3
***n*-C_{96}**	0.0051	0.0019	0.0027	1575.7

β in $m^2 \cdot (mol/s)/cm^3 \cdot K^{1/2}$ and V_D in cm^3/mol.

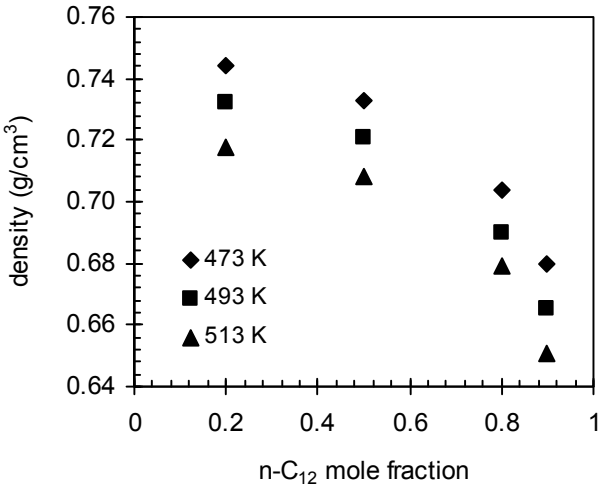

Fig. S1. Simulated density of *n*-C_{12} – *n*-C_{96} mixture as a function of *n*-C_{12} mole fraction.

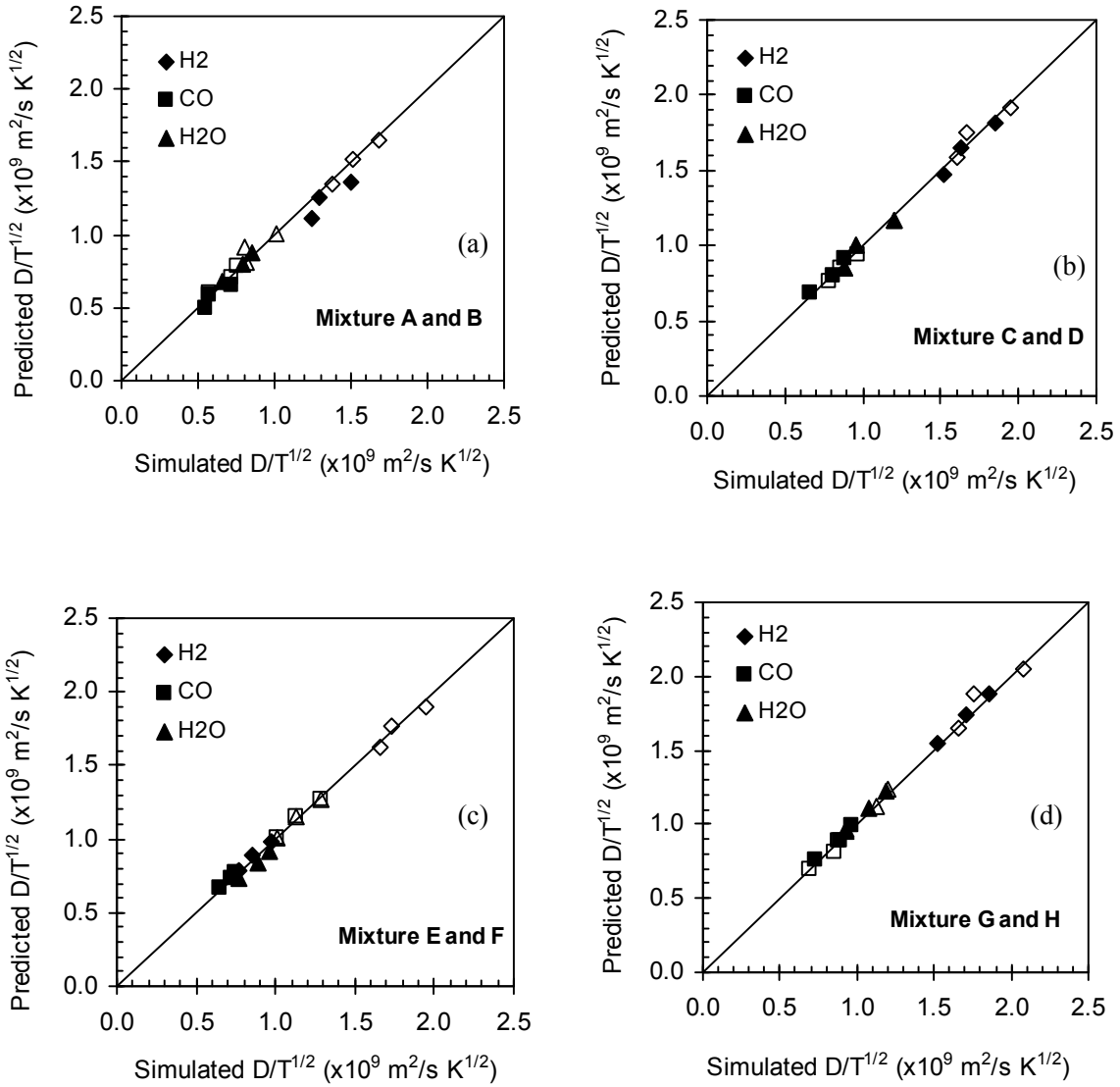

Fig. S2. Molecular simulation data and RHS theory correlations for the diffusivities of H_2, CO and H_2O in (a) mixture A (close symbols) and B (open symbols), (b) mixture C (close symbols) and D (open symbols), (c) mixture E (close symbols) and F (open symbols) and (d) mixture G (close symbols) and H (open symbols).