Impact of super-critical CO_2 on water/oil interfacial tension: A molecular dynamics case study

Yannick Agbor* and Barco Yolo

University of North Dakota, Department of Petroleum Engineering

***Corresponding author:** Yannick Agbor, University of North Dakota, Department of Petroleum Engineering, E-mail: yannick_agbor@yahoo.com

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Methodology

Ba/ 18 (2016) ( ) 1.1, F 1.1. A E G MAC / M 293K 4 . ACKM L 4 1 E (ME) 1.2 M (B ., 2007) B

2 HAKE . M E (ME) 12-6 L -J

$$E_{vdW} \mid D_0 \left(2 \left(\frac{R_0}{R} \right)^{12} - 4 3 \left(\frac{R_0}{R} \right)^{6} \right) \quad (4.1)$$

D_0 L -J ,

D 0 0

F 1.3 - C 2 C 2 +C 2

A F 1.3, A C 2 IF . (F 1.3 1.3). IF C 2 5, 10

(L -L ., 2008)

$$\nu/t() \mid \left|(P_{nn}/n,t()4\,P_{tt}/n,t()d_n \right. \quad (4.3)$$

P P P. $\gamma(t)$ 7 252 53 J (,)-229.2- 9 87 9 3( )9 09

Table 1.2: Interfacial tension between liquid and vapor phases of pure hydrocarbons at 68Á F and 14.7 psi.

Component	5P1P simulation	Error	5P1P± Experiment[a,c]
Propane	9.85	0.302	10.1
Butane	13.3	0.23	12.46
Pentane	16.02	0.1	15.82
Hexane	18.41	0.12	18.43
Heptane	20.25	0.07	20.14
Octane	21.57	0.05	21.62

a* surface-tension. c* Froba et al, 2003

Table 1.3: Interfacial tension between liquid and vapor phases of pure hydrocarbons at 68Á F and 14.7 psi.

Component	[illegible] simulation	Error	[illegible] Experiment[b]
Propane	502.4	0.19	498
Butane	579.2	0.019	579
Pentane	627	0.045	626
Hexane	659	0.035	659.4
Heptane	684.1	0.048	683.7
Octane	705	0.059	703

b* engineering toolbox/ density/ alkanes