

SUPPORTING INFORMATION

Title: Modeling of chemical equilibrium and gas phase behavior for the direct synthesis of dimethyl carbonate from CO₂ and methanol

Authors: Felipe Bustamante, Andrés F. Orrego, Sebastián Villegas, Aída L. Villa

Corresponding Author: Felipe Bustamante

Sede de Investigación Universitaria, SIU

Calle 62 #52-69 Torre 2 - Lab 332

Medellín-Colombia

e-mail: fbustama@udea.edu.co

Phone (574) 2198535

Fax (574) 2196565

Postal Code 1226

The available supporting information includes the following: a) results of average absolute deviations (AAD%) of pressure and vapor phase composition for six binary subsystems; b) 2D views of Figure 14 in order to facilitate its use: the figures show P vs T curves for various CH₃OH/CO₂ feed ratios..

Table S-1 Average absolute deviations (AAD%) for dew pressures and vapor phase compositions.

Binary System	T/K	P/bar	Number of points	ADD (%)	
				$\Delta P/P$	$\Delta y/y$
CO ₂ + Methanol	291.15	5.6 - 23.6	6	19.0	0.2
	298.15	9.2 - 26	6	11.4	0.1
	303.15	8.9 - 34.2	7	10.7	0.1
	308.15	13.2 - 48.7	9	9.6	0.1
	313.15	13.2 - 45.6	8	7.6	0.1
	323.15	10.3 - 38.6	3	16.7	0.5
	348	14.5 - 34.9	5	2.3	0.2
CO ₂ + DMC	303.15	2.4 – 40.7	5	25.4	0.2
	310.15	3.9 – 30.5	4	23.5	0.3
	323.15	2.9 – 42.8	5	24.6	1.0
	333.15	6.1 – 33.8	3	26.6	0.3
CO ₂ + Water	298.15	0.81 - 18.9	10	25.9	0.1
	323.15	4.4 - 26.0	8	22.7	0.6
	348.15	11.1 - 31.3	5	13.7	0.2
	373.15	23.0 - 36.8	5	14.6	0.4
	393.15	12.9 - 50.4	6	9.4	0.8
Methanol + Water	298.15	0.035 - 0.164	10	6.9	14.7
	312.91	0.071 - 0.347	21	2.8	8.0
	322.91	0.119 - 0.551	20	1.2	6.7
	333.15	0.198 - 0.846	22	0.3	1.1
Methanol + DMC	337.35	0.41-0.99	14	7.6	23.7
	377.15	1.54-4.0	13	3.6	4.8
	391.15	2.29-6.05	13	1.51	2.04
	411.15	3.82-10.42	13	4.03	7.2
	428.15	5.66-15.66	13	1.87	4.23
DMC + Water	P/KPa	T/K	Number of points	$\Delta T/T$	$\Delta y/y$
	101.3	351,5 - 364,8	5	0.1	4.2

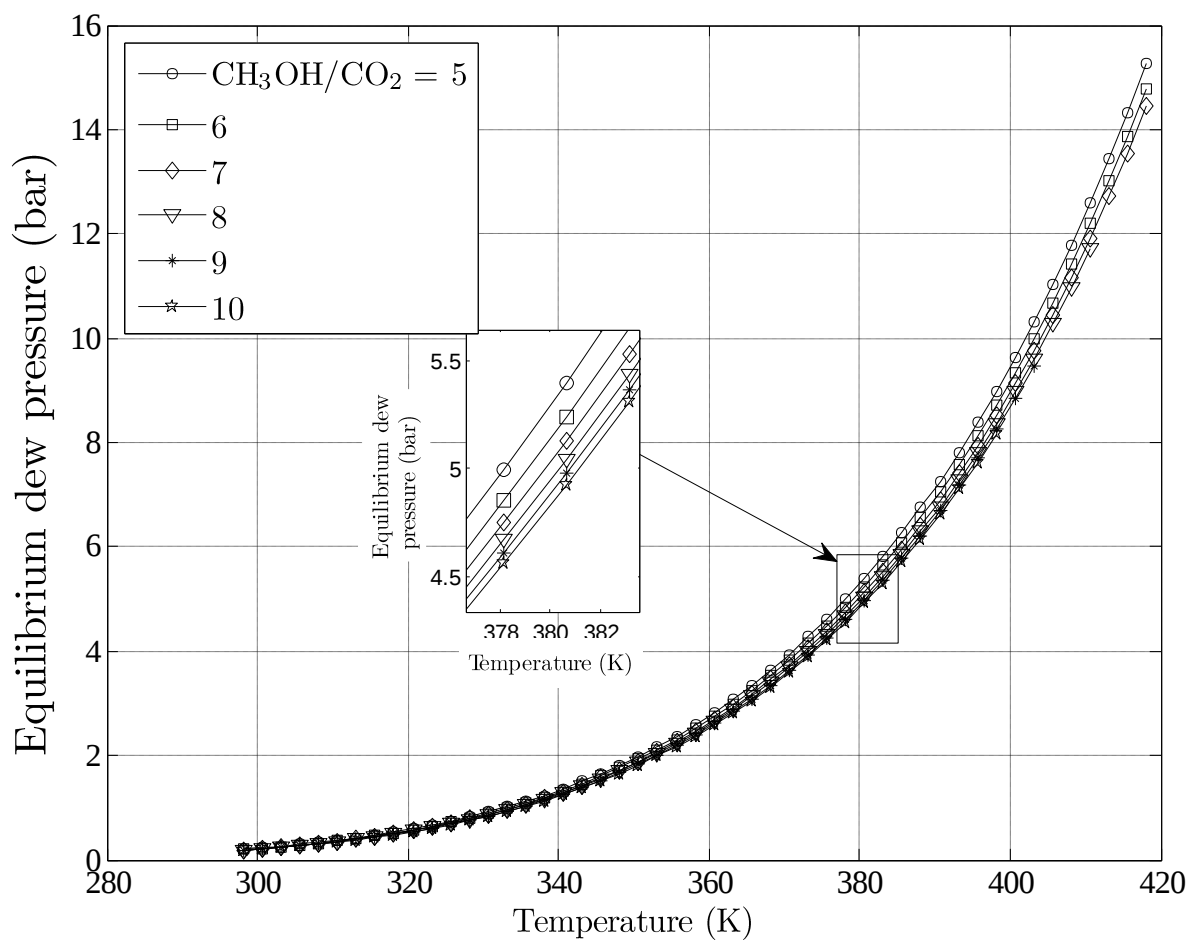


Figure S-1. P-T view of figure 14 for large values of $\text{CH}_3\text{OH}/\text{CO}_2$

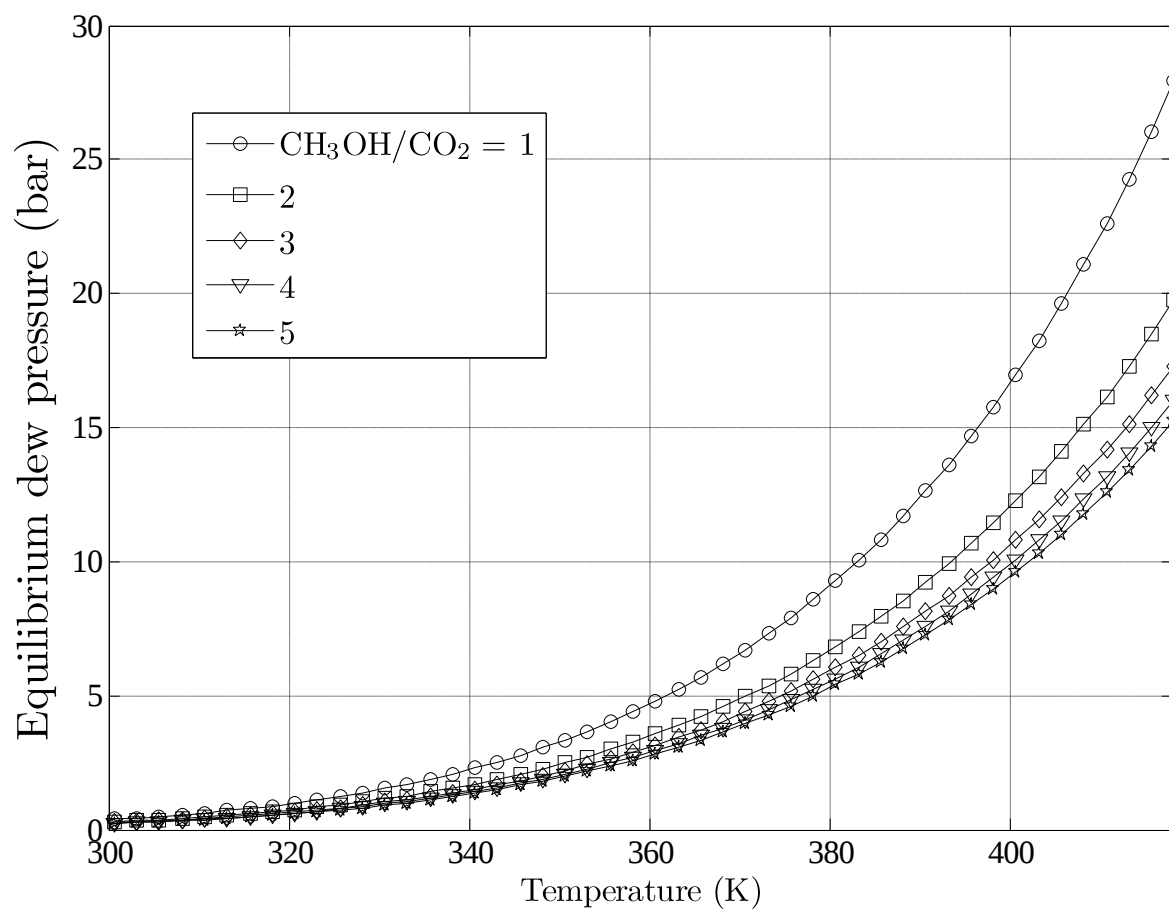


Figure S-2. P-T view of figure 14 for intermediate values of $\text{CH}_3\text{OH}/\text{CO}_2$

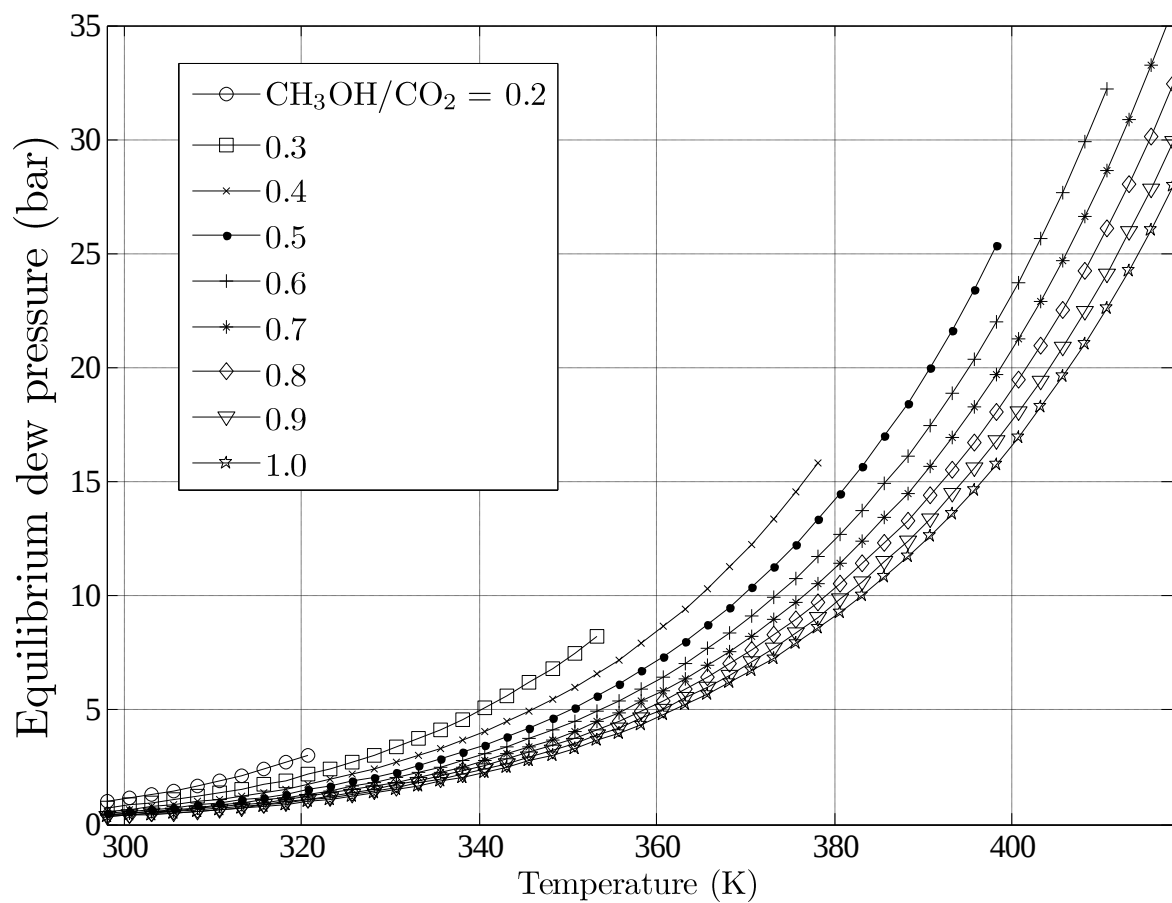


Figure S-3. P-T view of figure 14 for small values of $\text{CH}_3\text{OH}/\text{CO}_2$