

Electronic Supplementary Information Heat of capillary condensation in nanopores: New insights from equation of state

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Parachors were correlated according to:

$$\phi = \sum_{k=1}^{10} p_k ({}^{10} \log(T_C - T))^{k-1} \quad (S1)$$

where T_C is the critical point and p_k is the correlation coefficients fitted to the data of surface tension up to temperatures close to the critical point. The data used for most fluids are taken from NIST webbook [1], except for acetone, which was taken from Vargaftik [2]. Table S1 contains the coefficients p_k for all fluids used in paper. The parachor in Eq (S1) has the unit of $[dn^{\frac{1}{4}} cm^{\frac{11}{4}} / mol]$.

Table S1. Coefficients p_k of Eq (S1) and the critical point T_C in [K]

	Argon	N ₂	O ₂	CO ₂	H ₂ O	pentane	hexane	acetone
p_1	61.091743	68.495557	63.520438	85.580976	59.876347	262.293739	389.326093	131.260641
p_2	-5.159504	-6.245909	-7.114718	-5.241881	-5.48561	-29.983511	-200.30909	36.100545
p_3	-0.201051	-0.770175	0.016529	-0.818488	-1.461685	26.247637	84.015175	-9.747544
p_4	-0.391738	0.854315	-1.094663	0.087605	7.058836	-22.764271	38.57336	0
p_5	0.341847	-0.397066	2.092429	0.113607	-2.969046	8.070634	-17.300689	0
p_6	0.050105	-0.228211	-0.698482	0.085272	-6.122237	-5.845499	-51.945727	0
p_7	0.086816	0.641969	-1.001154	0	6.91992	10.708881	61.164811	0
p_8	-0.037114	-0.206024	1.013343	0	-2.615132	-8.674332	-30.463338	0
p_9	0	0	-0.249607	0	0.344466	3.179411	7.72089	0
p_{10}	0	0	0	0	0	-0.441403	-0.817504	0
T_C	150.687	126.192	154.581	304.1282	647.096	469.7	507.82	508

Due to the change in the parachor correlations, the parameter λ is refitted as:

$$\lambda = \sum_{i=0}^3 \sum_{j=0}^2 b_{ij} T^i r_p^{j-1} \quad (S2)$$

The coefficients b_{ij} are listed in Tables S2 and S3 for all confined fluids used in this paper. If not listed in the tables, $b_{ij} = 0$. The listed references contain the experimental capillary-condensation pressure from which the parameter λ is derived.

Table S2. Coefficients b_{ij} of Eq (S2) for fluids in a single size pores.

	2.2-nm MCM-41 (for pentane: $r_p = 2.285$ nm)						1.6-nm MCM-48	
	Argon	N ₂	O ₂	CO ₂	pentane	hexane	hexane	acetone
b_{01}	0.192918	2.810056	3.893866	-0.415885	0.0517499	1.3188768	-1.909683	0.299824
b_{11}	0.002054	-0.078271	-0.097196	0.0039051	0.0010137	-0.006387	0.010616	-3.934E-4
b_{21}	2.1913E-5	8.7502E-4	8.7956E-4	2.4675E-6	2.14E-6	1.1341E-5	-9.6219E-6	3.4876E-6
b_{31}	0	-2.9196E-6	-2.4058E-6	0	0	0	0	0
Ref	[3]	[3]	[3]	[3]	[4]	[5]	[6]	[6]

Table S3. Coefficients b_{ij} of Eq (S2) for fluids in multiple size pores.

	MCM-41 87 K	SBA-15	MCM-41 298.2 K
	Argon	N ₂	H ₂ O
b_{00}	2.71417424	0	1.025
b_{10}	-0.018012	0	-0.001584
b_{20}	0	0	0
b_{01}	-1.482267	-2.4818556	-1.5735
b_{11}	0.016473	0.05898146	0.003977
b_{21}	0	-0.0002487	0
b_{02}	0	0.98629802	0
b_{12}	0	-0.0220987	0
b_{22}	0	0.00011318	0
Ref	[7]	[8]	[9]

References

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