Supporting Information

Surface Modification of Mesostructured Cellular Foam to Enhance Hydrogen Storage in binary THF/H_2 Clathrate Hydrate

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Table S1. Regressed values of rate constants (k), Avrami exponent (n) from the JMAK[1] model.

System	T (K)	JMAK		AAD
		k (min^{-1})	n	
f-1	268	0.065	0.20	0.68
	265	0.092	0.18	0.84
	262	0.092	0.29	0.74

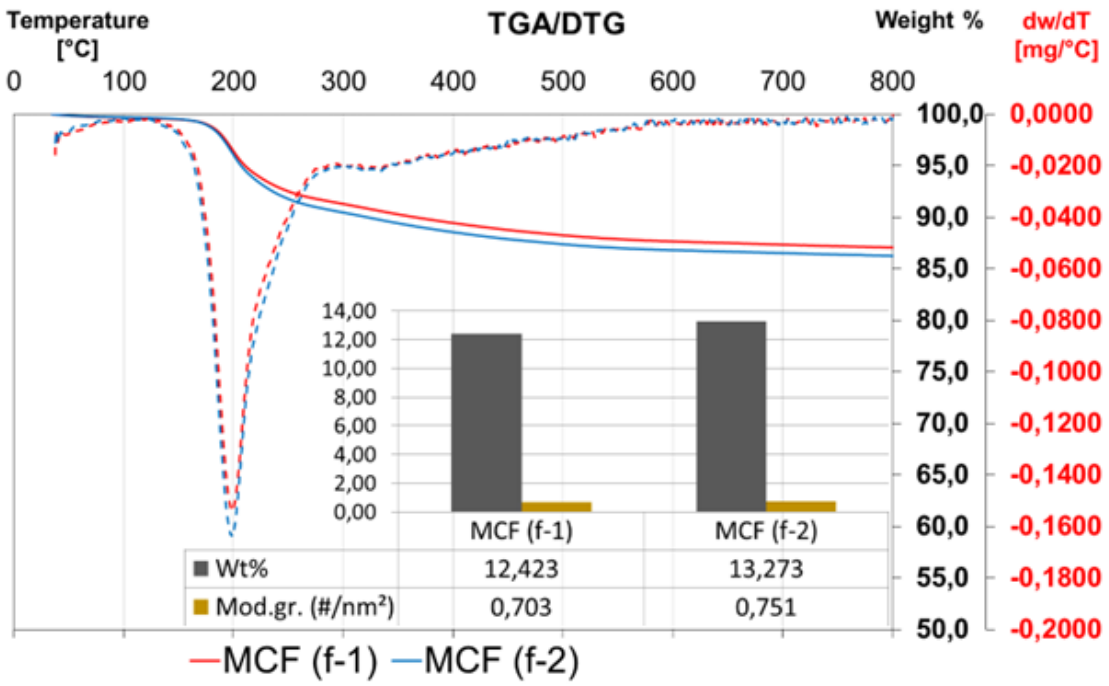


Figure S1. Thermogravimetric analysis and estimation of the group's modifier/nm2 (Mod.gr., #/nm^2) resulted from the corroboration of carbon content after 423 K (150° C) and BET surface area.

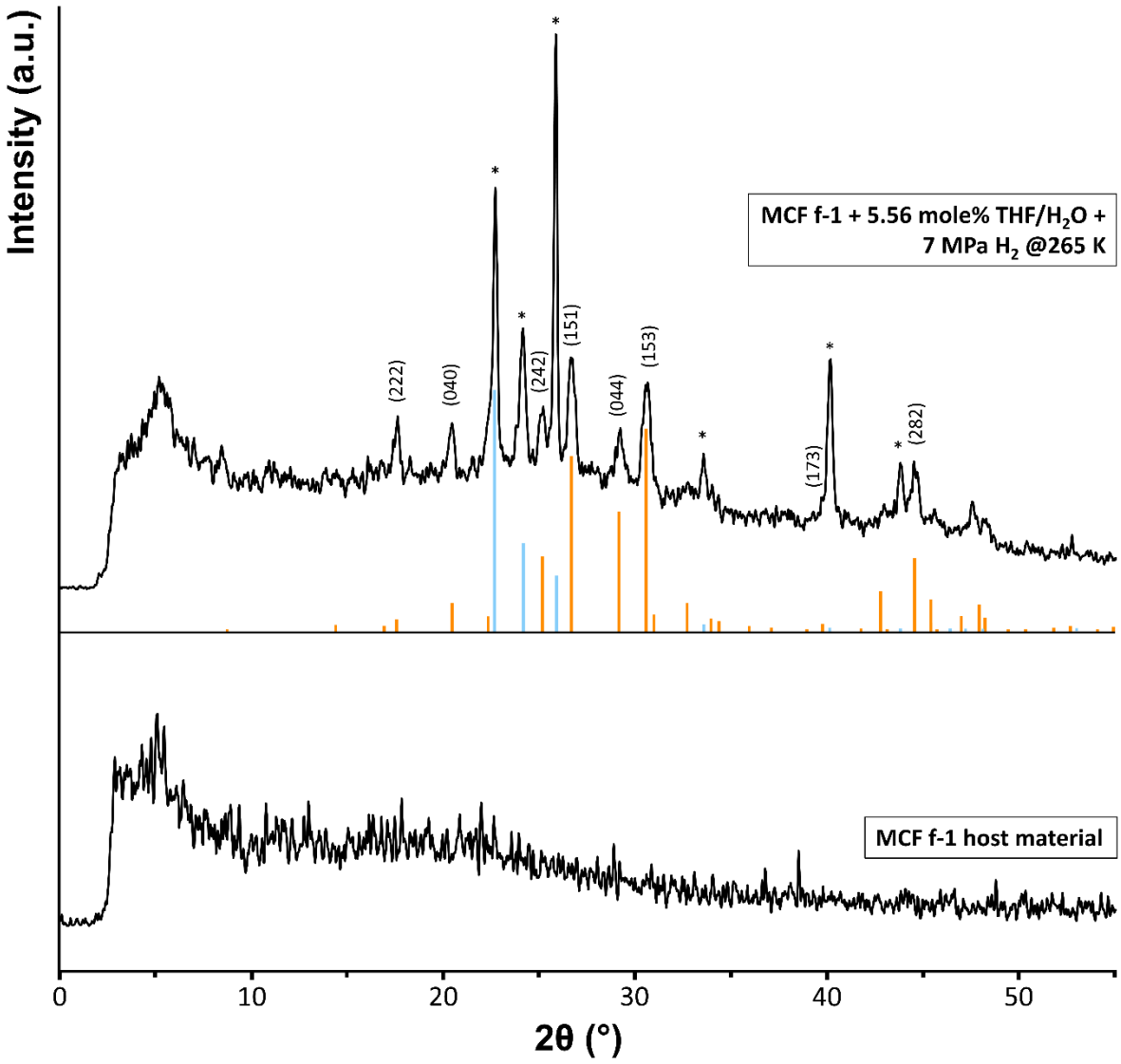


Figure S2. X-ray diffraction pattern of MCF f-1 saturated with 5.56 mole% THF/H_2O solution (100 % pore volume) subjected to 7.0 MPa H_2 pressure at 265 K, determined under cryogenic conditions. Reflections characteristic of sII clathrate hydrates (Fd-3m; a = 17.3 Å) are denoted by their corresponding miller indices (hkl). Reference diffraction lines for sII hydrates and hexagonal ice are shown in orange and blue, respectively [2]. The presence of hexagonal ice (marked with an asterisk (*)) is exacerbated when using liquid nitrogen as refrigerant, as it promotes water condensation and subsequent ice formation from water vapor in the air. **Bottom**. Reference X-ray diffraction pattern of the porous host material, i.e., MCF f-1 (dried).

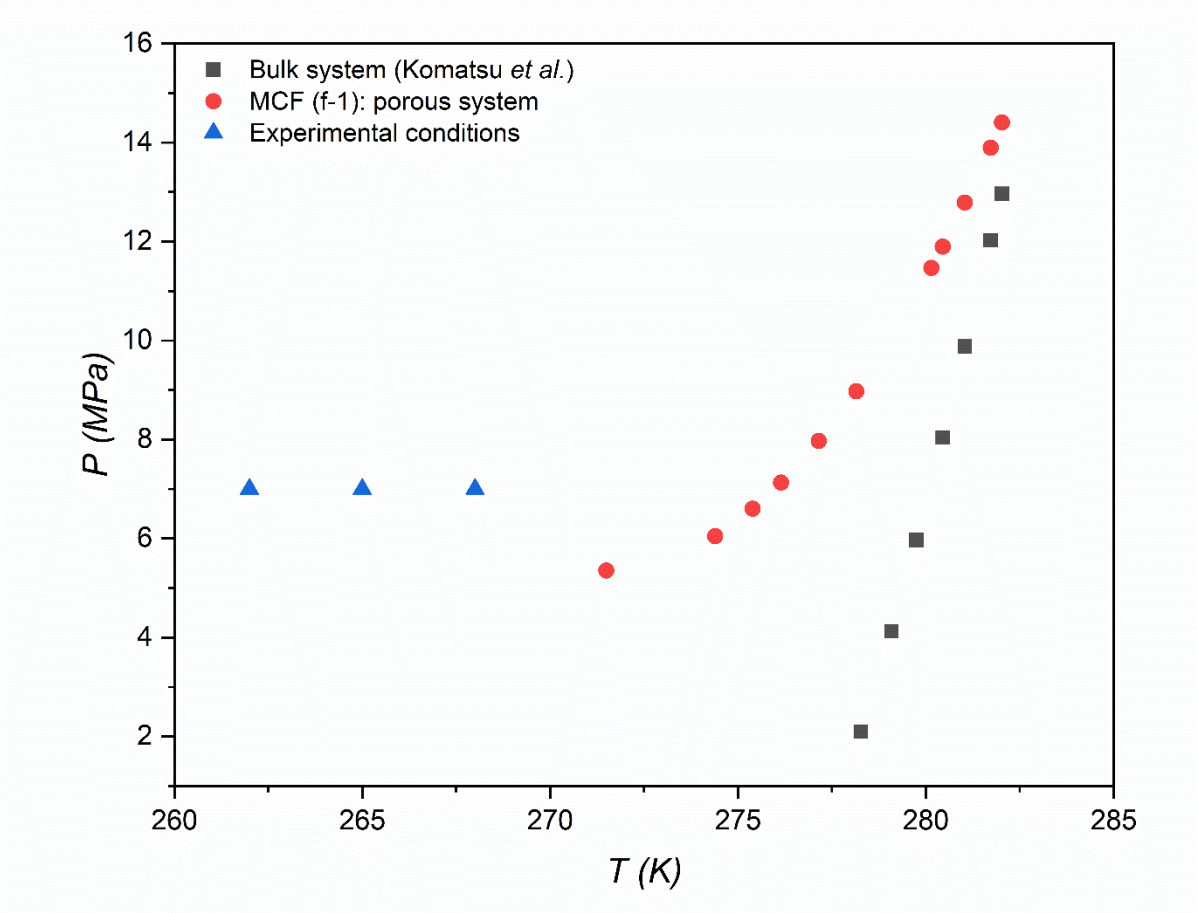


Figure S3. Phase equilibrium of binary H_2-THF hydrate in the presence of porous and bulk systems [3]. The blue triangles represent the experimental conditions used in this work.

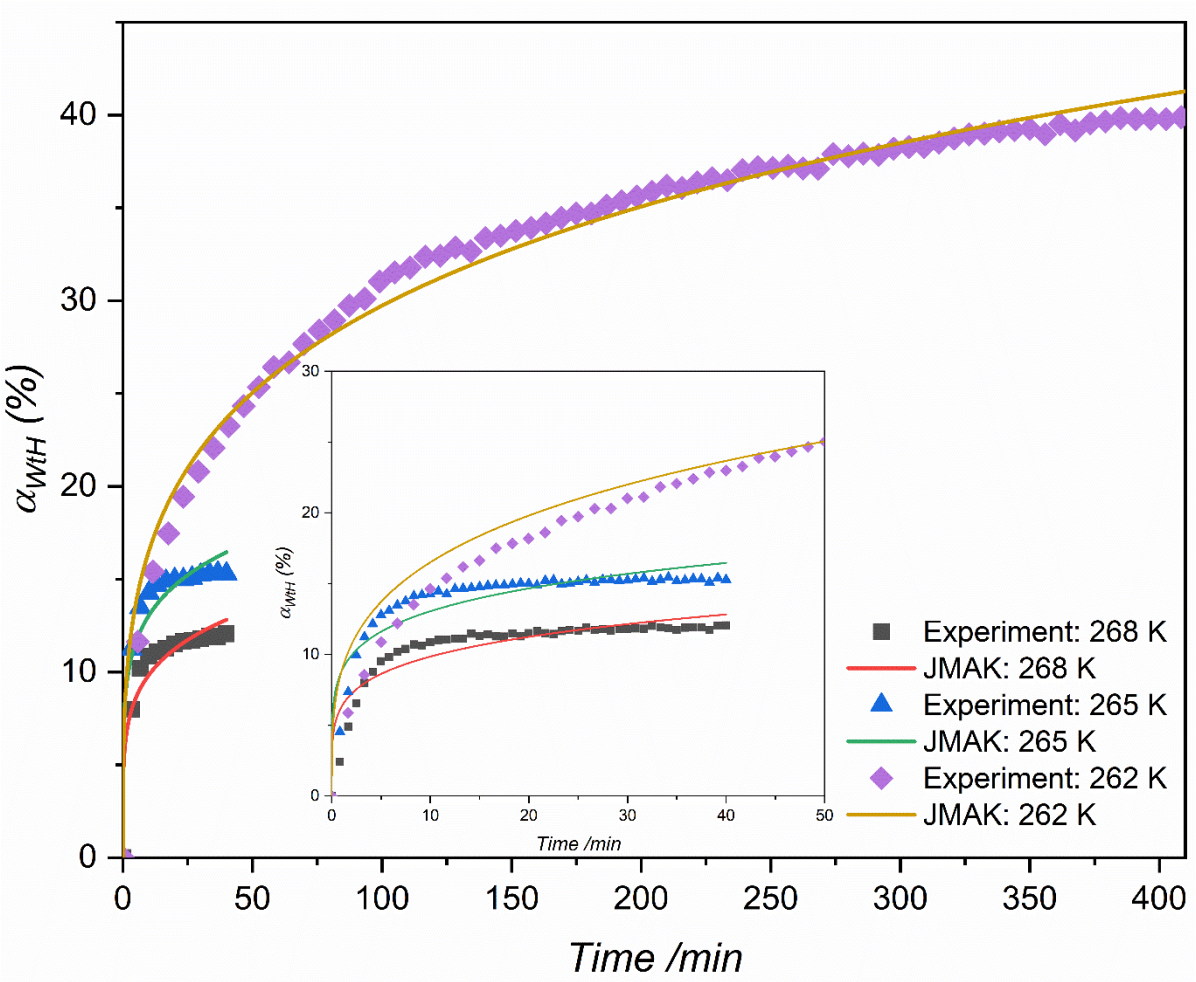


Figure S4. Comparing the JMAK model[1] to experimental data for water-to-hydrate conversion (%) in THF-like functionalized MCF (f-1) porous material at three different temperatures with an initial pressure of 7 MPa.

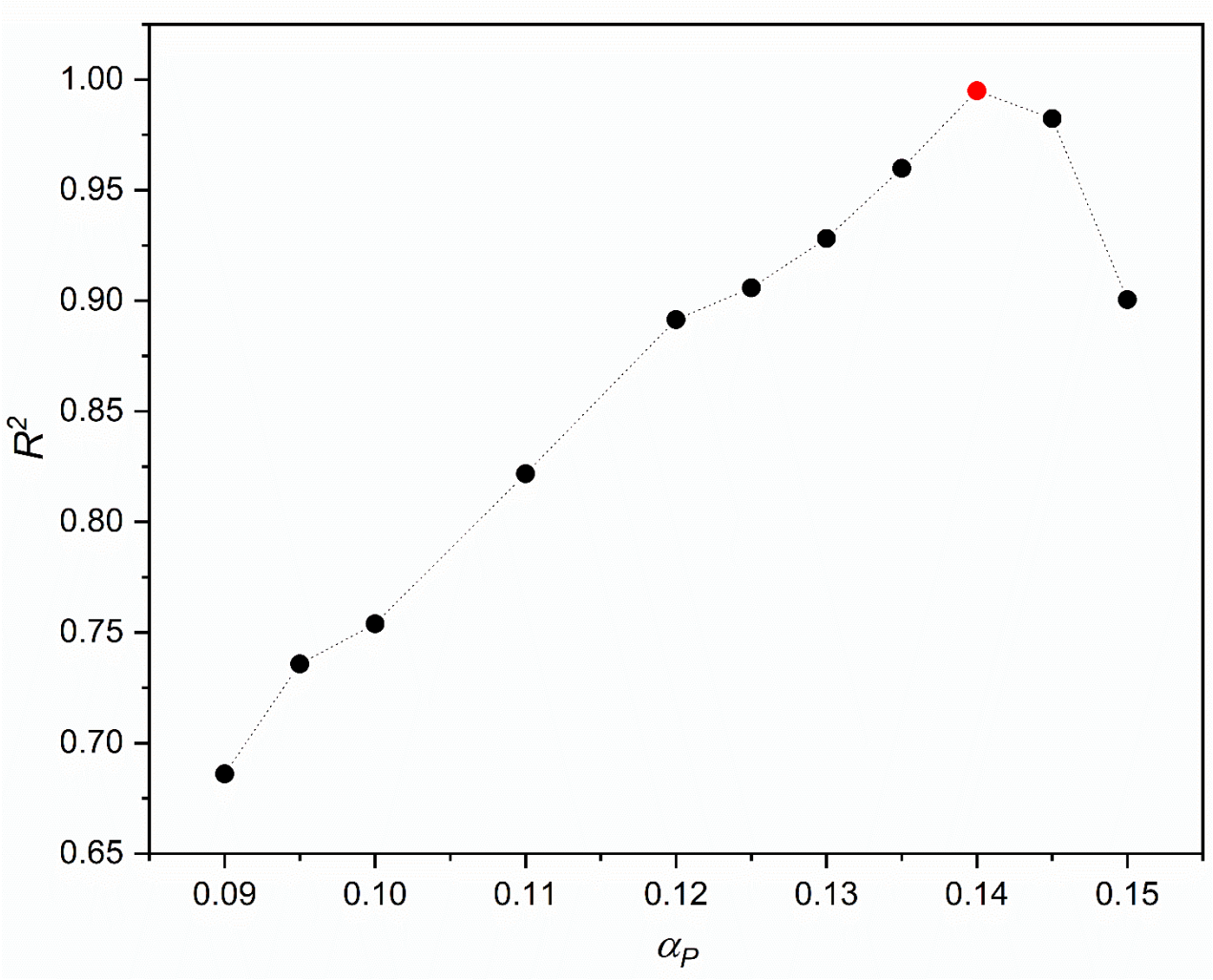
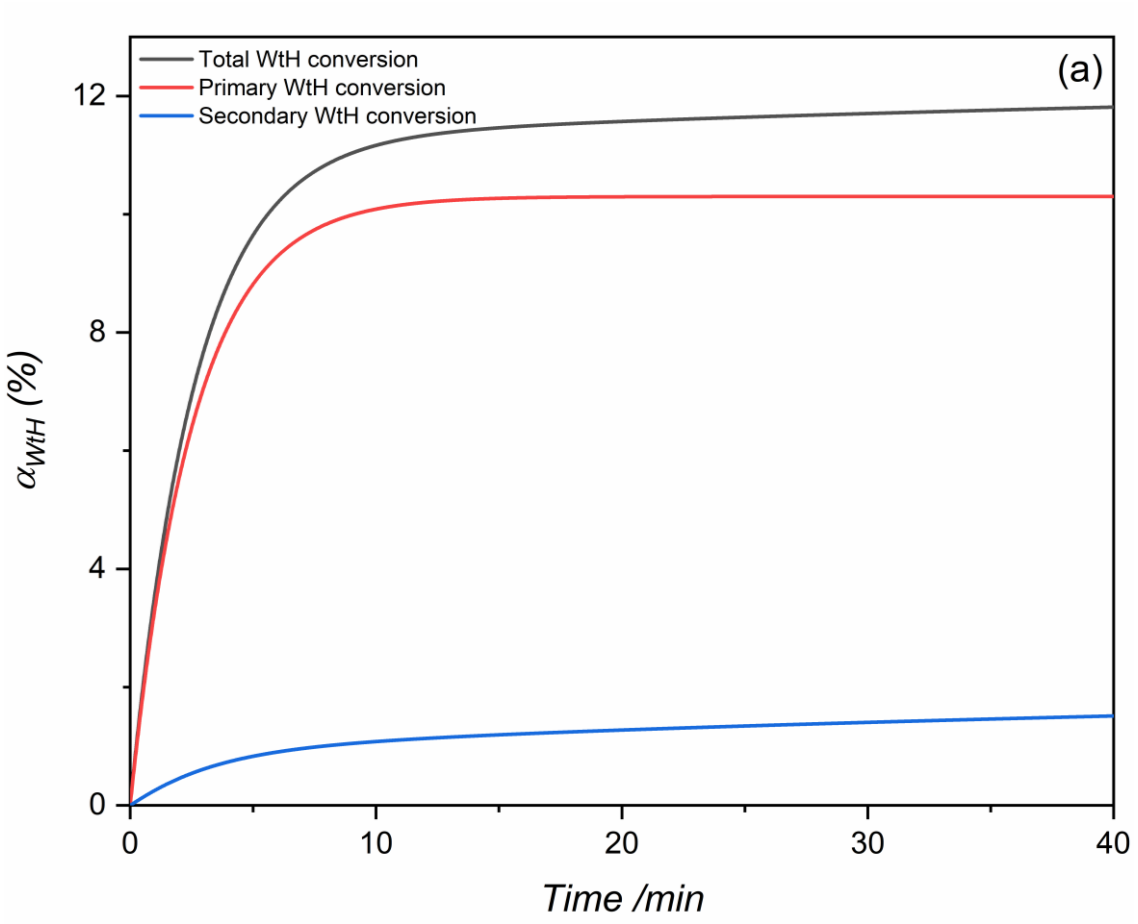
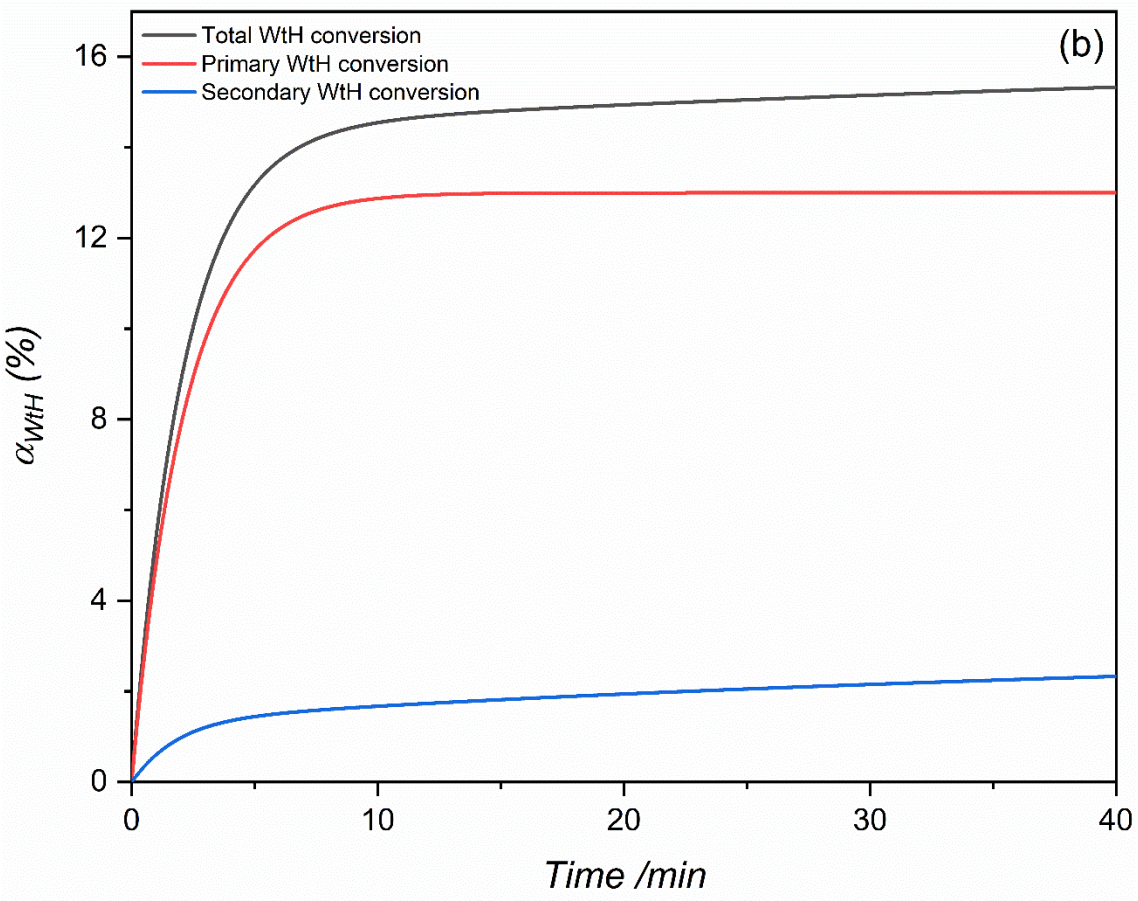


Figure S5. Effect of changing α_P on the degree of fit for the material MCF (f-1) at 265 K.


Total WtH conversion
Primary WtH conversion
Secondary WtH conversion
(a)
12
8
4
0
α_{WtH} (%)
0
10
20
30
40
Time /min


Total WtH conversion
Primary WtH conversion
Secondary WtH conversion
(b)
16
12
8
4
0
α_{WtH} (%)
0
10
20
30
40
Time /min

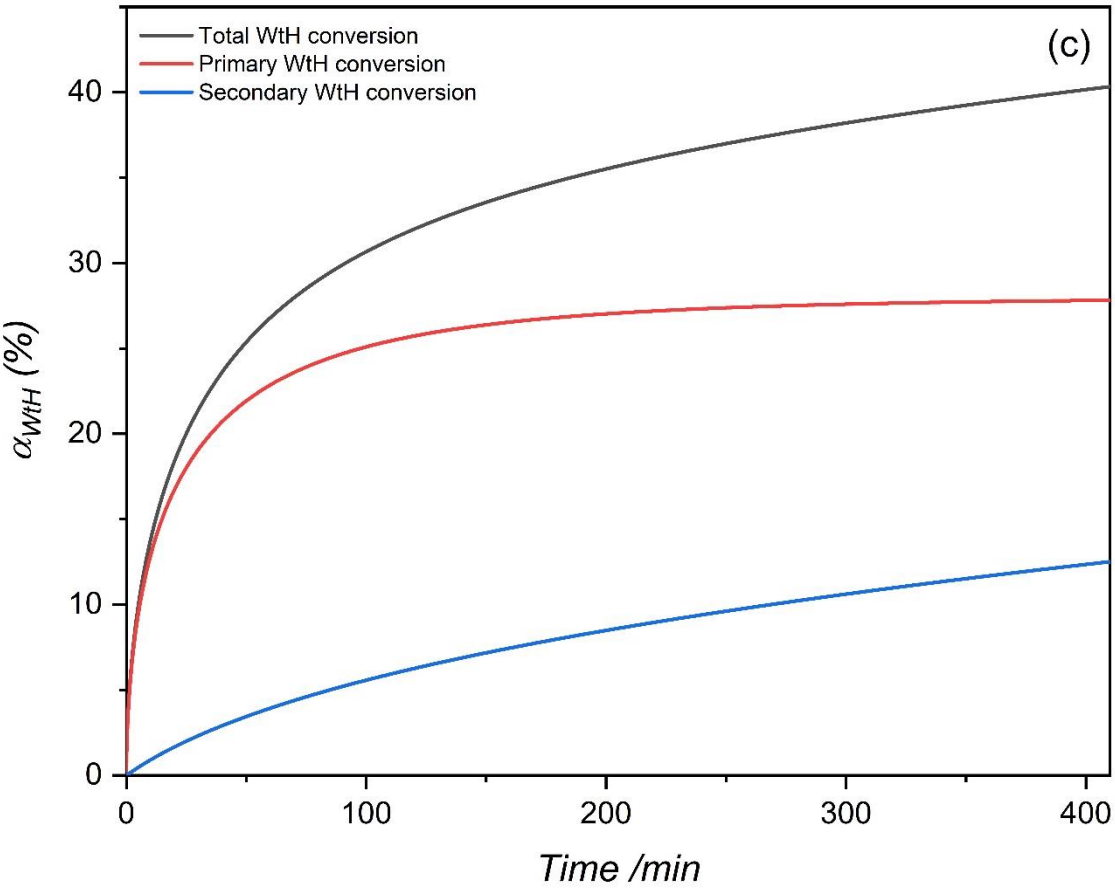


Figure S6. The contribution of primary and secondary-stage hydrate growth on water-to-hydrate conversion in material (f-1) at 268 K(a), 265 K(b), 262 K(c).

References

[1] M. Fanfoni, M. Tomellini, The Johnson-Mehl-Avrami-Kohnogorov model: A brief review, Il Nuovo Cimento D 20 (1998) 1171-1182.

[2] Y-H. Ahn, B. Lee, K. Shin, Structural Identification of Binary Tetrahydrofuran + O_2 and 3-Hydroxytetrahydrofuran + O_2 Clathrate Hydrates by Rietveld Analysis with Direct Space Method, Crystals, 8 (2018) 328.

[3] H. Komatsu, H. Yoshioka, M. Ota, Y. Sato, M. Watanabe, R. L. Smith, Jr, C. J. Peters, Phase Equilibrium Measurements of Hydrogen−Tetrahydrofuran and Hydrogen−Cyclopentane Binary Clathrate Hydrate Systems, J. Chem. Eng. Data, 55 (2010) 2214–2218