SUPPLEMENTARY MATERIAL

The influence of particle composition upon the evolution of urban ultrafine diesel particles on the neighbourhood scale

Irina Nikolova, Xiaoming Cai, Mohammed Salim Alam, Soheil Zeraati-Rezaei, Jian Zhong, A. Rob MacKenzie and Roy M. Harrison

Here we present details of the input parameters used in the box model simulations (Section S1) and some results (Section S2). All figures and tables are given in the Appendix.

S1. Model input parameters - size distribution, vapour pressures, modal composition mass fractions in the nucleation and Aitken modes, gas-phase ambient concentrations.

The initial size distribution is based on the measurements of Dall'Osto et al. (2011) and it is plotted in Figure 1-S. This ultrafine size resolved distribution represents the typical street canyon size distribution found next to a traffic site in Marylebone road in London (UK). The distribution has a well defined nucleation mode (particles with a diameter around or less than 30 nm) with a peak number concentration at ~ 23 - 24 nm. The Aitken mode (particles with diameter between 30 and 100 nm) is seen as a shoulder attached to the nucleation mode with a centre between 50 - 60 nm. Dall'Osto et al. (2011) show that the observed size distribution is subject to a major transformation caused by extensive evaporation of volatile material from the particles. The diameter of the nucleation mode particles decreased during the transport of the particles between the street canyon and the nearby city park over a distance of about 665m, as shown in Figure 1-S in the Appendix. The nucleation-mode peak diameter, $D_{pg,nuc,}$ corresponding to the highest number concentration in the nucleation mode, was found at around 8 – 9 nm. In our study, we aim to put forward a realistic set of compositions and thermodynamic properties that could explain this diameter decrease as seen in the observations. Chemical analyses during the observations are missing; however, there are some laboratory data pointing to the nature of organics that participate in the composition from emitted particles collected from an engine testbed (Alam et al., 2016). Figure 2-S shows the normalised mass concentration per compound in the range [$C_{16}H_{34}$:$C_{32}H_{66}$] for a given size class. Particles in the Nucleation and Aitken modes consist of about 10% and higher contribution from compounds in the range $C_{25}H_{52}$-$C_{29}H_{60}$.

In our modelling study the UFP size-resolved mass composition per mode (eq. 1) is initialised as follows. The mass of a particle, M_{ij}, per size bin *i* and compound *j* in the range [$C_{16}H_{34}$:$C_{32}H_{66}$] is expressed as

$$M_{ij} = \sum_{k=1}^{2} \frac{\pi}{6} Dp_i^3 \rho X_{jk} N_{ik} \qquad \text{(eq. 1)}$$

i = 1,..., 15 – number of size bins

j = 1,..., 18 – indices [1-17] correspond to surrogate n-alkane compounds in the range $C_{16}H_{34}$ – $C_{32}H_{66}$; index 18 refers to the involatile core

k = 1, 2 - particle mode, where 1 = Nucleation mode, 2 = Aitken mode

Dp_i – particle diameter per size bin *i*, m

M_{ij} – size resolved mass per size bin i and per compound *j*, kg m^{-3}

ρ = 1000 kg m^{-3}, particle density, held constant to avoid introducing highly uncertain parameters for density of involatile core.

X_{jk} – fraction of mass in a particle in mode *k* per compound *j*

π = 3.14

is the number of particles per bin width ΔDp, [# m^{-3}]. The number log-normal size distribution (eq. 2) is given as follows:

$$n(Dp)_{ik} = \frac{N_k}{\sqrt{(2\pi)}\, Dp_i \ln(\sigma_{gk})} \exp\left(-0.5\left(\frac{\ln(Dp_i / Dp_{gk})}{\ln(\sigma_{gk})}\right)^2\right) \qquad \text{(eq. 2)}$$

N_k = 3.0x10^{10} and 1.8x10^{10} (# m^{-3}) are the total number concentrations in the Nucleation and Aitken mode, respectively

Dp_{gk} = 23 and 65 nm are the geometric mean diameter in the Nucleation and Aitken mode, respectively

σ_{gk} = 1.6 is the geometric standard deviation for both modes

The fraction of mass X_{jk} of each particle in a mode k per compound SVOC in the range $C_{16}H_{34}$-$C_{32}H_{66}$ is calculated (eq. 3) as follows:

$$X_{jk} = \frac{f(m_j, \sigma_{modal})}{\sum_{j=1}^{17} f(m_j, \sigma_{modal})} (xx_{jk} - sf_k) \qquad \text{(eq. 3)}$$

where $f(m_j,\sigma_{modal})$ is the modal composition in the form of a Gaussian distribution (eq. 4), xx_{jk} is SVOC composition given by the Gaussian parameterisation (eq. 5), and sf_k is the solid involatile fraction per mode *k*:

$$f(m_j, \sigma_{modal}) = \frac{1}{\sqrt{2\pi}\,\sigma_{modal}} \exp\left(-0.5\left(\frac{x_j - m_j}{\sigma_{modal}}\right)^2\right) \qquad \text{(eq. 4)}$$

$$xx_{jk} = \sum_{j=1}^{17} \frac{f(m_j, \sigma_{modal})}{\sum_{j=1}^{17} f(m_j, \sigma_{modal})} = 1 \qquad \text{(eq. 5)}$$

σ_{modal} = 1,..., 5 – standard deviation of modal composition

x_j = 1, … , 17 – number assigned to the SVOC compound

m_j = 1, …, 17 – modal composition compound for each SVOC in the range $C_{16}H_{34}$-$C_{32}H_{66}$

In this study the role of an involatile core (sf_k) is evaluated, too, by considering an involatile core to be 1%, 5% and 10% of the mass in a particle in the Nucleation mode (k = 1). Input modal composition mass fractions in the nucleation mode and composition standard deviation are presented in the Appendix in Table 1-S, 2-S and 3-S for involatile core of 1%, 5% and 10%, respectively. The involatile core in the Aitken mode is 90% and the input modal composition mass fractions are given in Table 4-S in the Appendix.

Input vapour pressure parameterisations are given in Table 5-S. A-a, B-c and Co are used in this study to represent the uncertainties in the vapour pressure and evaluate the overall effect on the evaporative shrinkage of the nucleation mode particle diameter. Figure 3-S shows the ratio of vapour pressure between 298 K and 273 K for A-a, B-c and Co vapour pressure parameterisations and n-alkane compounds in the range $C_{16}H_{34}$-$C_{32}H_{66}$. The ratio for B-c and Co vapour pressure parameterisations is within an order of magnitude for compounds in the range $C_{16}H_{34}$-$C_{25}H_{52}$, however, it increases two to three orders of magnitude for higher molecular weight compounds. The ratio for A-a vapour pressure parameterisation is within an order of magnitude for compounds in the range $C_{16}H_{34}$-$C_{21}H_{44}$, and increases substantially for the remaining compounds. This would imply that for the selected timescale of 100 s there will be a shift in the threshold modal compositions to lower carbon-number compounds in comparison with the threshold modal compositions discussed in this study. The temperature dependence on evaporation is not considered further in this study but should be borne in mind.

The initial gas-phase concentrations for the n-alkanes in the range $C_{16}H_{34}$-$C_{32}H_{66}$ (Table 6-S) are as for the study in Nikolova et al. (2016) and are based on the roadside atmospheric measurements of Harrad et al. (2003).

S2. Results

Figure 4-S and Figure 5-S show the nucleation mode peak diameter $D_{pg,nuc}$ after 100 s using the vapour pressure parameterisations following Myrdal-Yalkowsky et al (1997, B-c) and Nannoolal

et al (2008, A-a), respectively. The nucleation mode particles consist of initial 1% non-volatile material. The threshold modal composition value changes from $C_{27}H_{56}$ for the B-c parameterisation (Figure 4-S) to $C_{22}H_{46}$ for A-a (Figure 5-S).

Figure 6-S shows the relative difference of the $D_{pg,nuc}$ between the highest (B-c) and lowest (A-a) vapour pressure parameterisations evaluated at 1 s, 10 s, 50 s and 100 s. Overall the largest difference is propagating to higher standard deviation sigma when simulation time increases as well as moving towards higher carbon-number modal compositions. In other words the relative differences become larger with time, pointing back to the huge differences in vapour pressure parameterisations between B-C and A-a. The choice of a particular vapour pressure dataset changes the range of carbon numbers by 2 in the first 10 seconds for which the highest relative difference is simulated. The 1-s relative difference is the highest for sigma 1 and modal compositions $C_{19}H_{40}$-$C_{21}H_{44}$. The 10-s highest relative difference has shifted to modal compositions $C_{21}H_{44}$-$C_{23}H_{48}$ and sigma = 1, 2. Higher relative differences (50% and more) are also simulated at sigma = 3. The 100-s relative difference is the highest for modal compositions $C_{22}H_{46}$-$C_{24}H_{50}$ and sigma = 1, 2, 3, but also relative differences of around 50% are simulated for sigma = 5.

Figure 7-S shows the '100-s effective involatile core' for the nucleation mode particles. Results are shown at 1%, 5% and 10% initial non-volatile material in the nucleation mode particles, modal compositions $C_{24}H_{34}$ and $C_{32}H_{66}$ and for various composition standard deviations, sigma. Vapour pressure parameterisations follow Myrdal and Yalkowski (1997; B-c in Table 1-S) and Nannoolal et al. (2008; A-a in Table 1-S). Figure 5-S presents the sensitivity to the non-volatile core in the nucleation mode for modal compositions $C_{24}H_{50}$ and $C_{32}H_{66}$ evaluated for B-c and A-a vapour pressure parameterisations. The 100-s effective involatile core for modal composition $C_{24}H_{50}$ and B-c vapour pressure parameterisation increases when the non-volatile core increases.

This is simulated for an increasing σ too, due the increasing number of lower volatility components that are added into the particle composition. The 100-s effective involatile core for modal compositions $C_{24}H_{50}$ (for A-a vapour pressure) and $C_{32}H_{66}$ (for A-a and B-c vapour pressures) shows an opposite trend with respect to sigma, i.e., the 100-s effective involatile core decreases due to the increasing number of higher volatility components added into the particle composition.

Acknowledgements

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Appendix

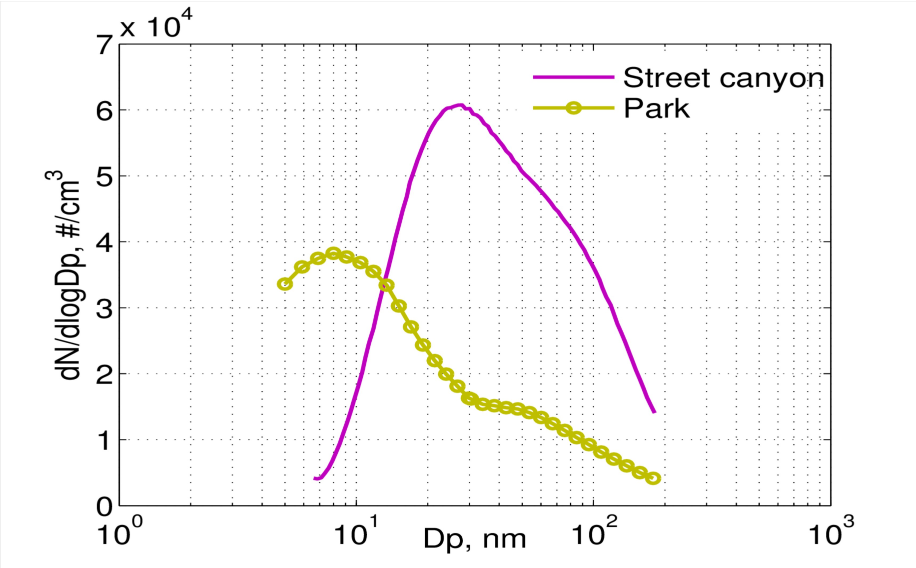

Figure 1-S. *Measured ultrafine particle size distribution in a street canyon (Marylebone Road, London, UK) and the nearby city park (Regents Park, London, UK).*

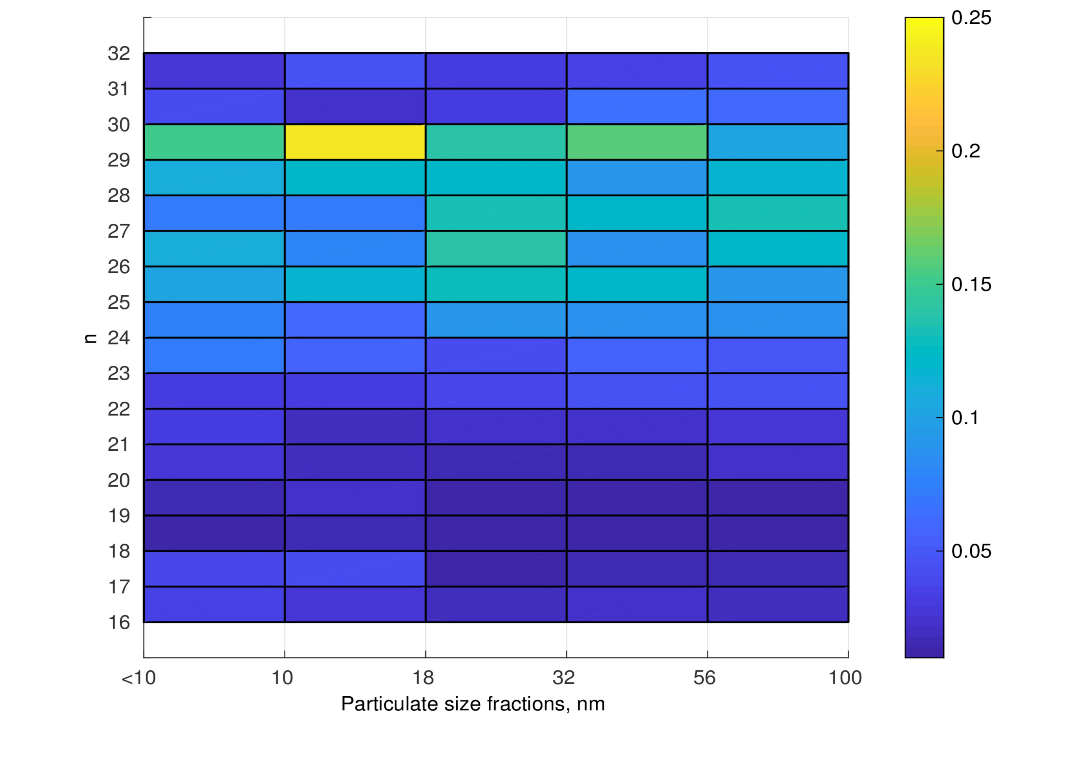

Figure 2-S. *Laboratory particulate mass fractions of n-alkanes $C_nH_{(2n+2)}$, where n=[16:32] for selected particulate diameter range [<10:100 nm]. Figure plotted based on the data presented in Alam et al. (2016).*

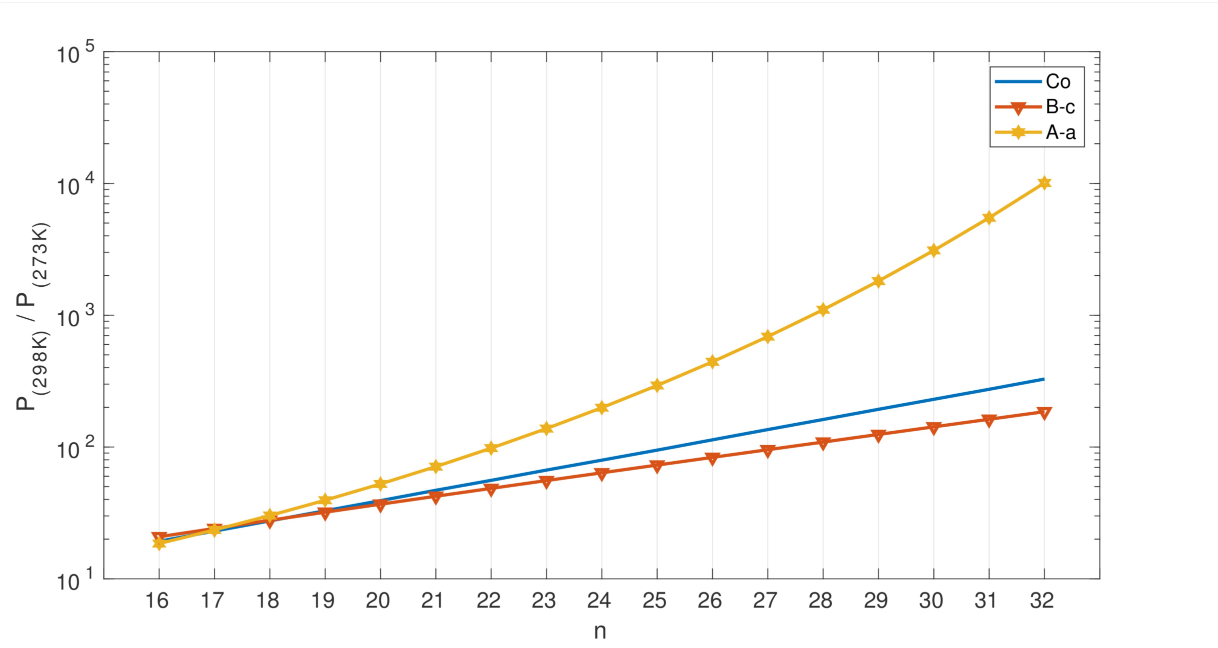

Figure 3-S. *Vapour pressure ratios for vapour pressure parameterisations A-a, B-c and Co and n-alkane compounds $C_nH_{(2n+2)}$, n=[16:32], between 298 K and 273 K.*

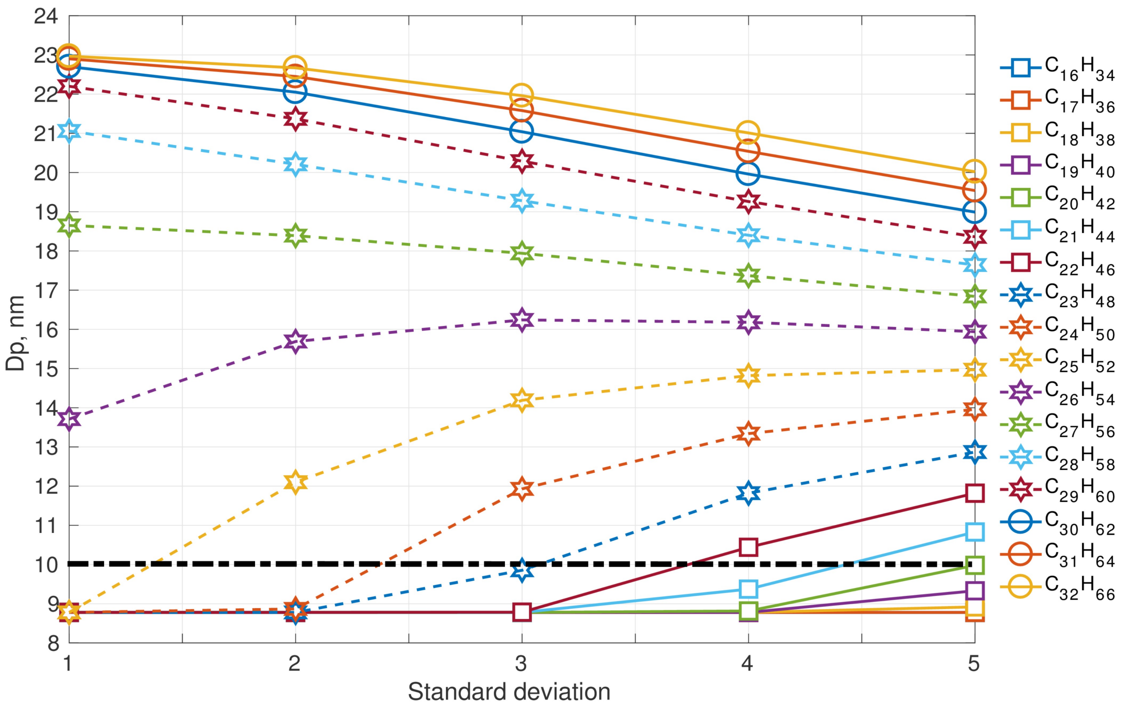

Figure 4-S. *Nucleation mode peak diameter Dp [nm] at 100 s of simulation depending on the modal composition and the composition standard deviation. The initial nucleation mode peak diameter is at 23 nm (not shown on the figure). Vapour pressure data follows Myrdal Yalkowsky et al. (1997, B-c). Initial nucleation mode particle involatile core is 1%.*

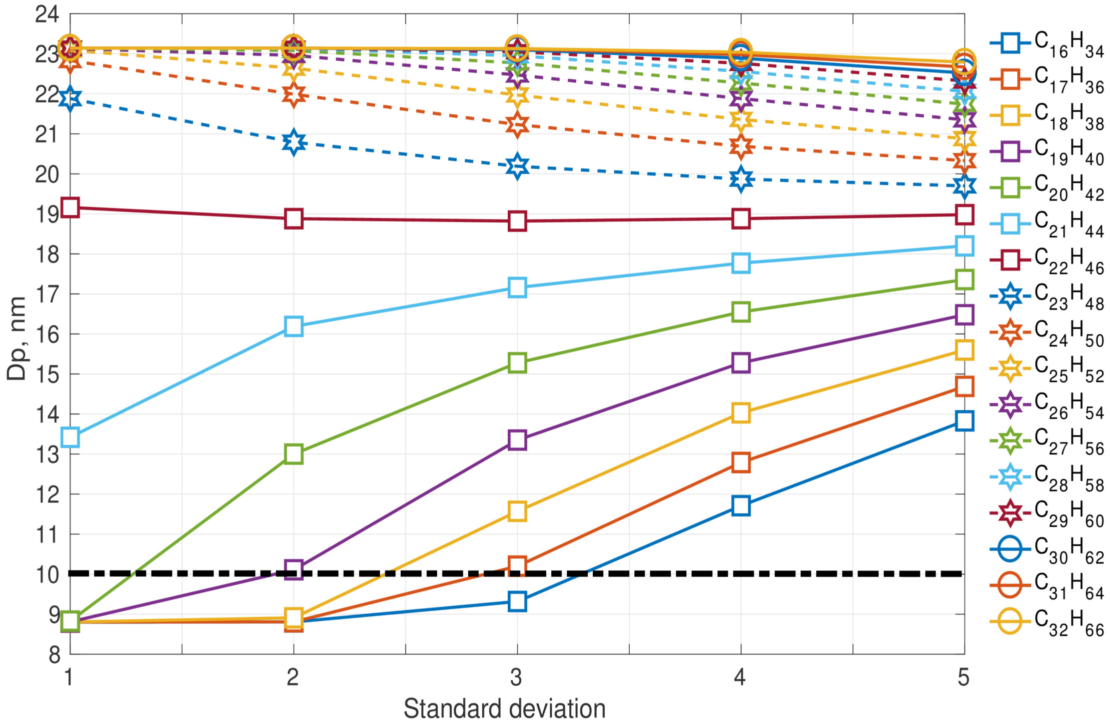

Figure 5-S. *Nucleation mode peak diameter Dp [nm] at 100 s of simulation depending on the modal composition and the composition standard deviation. The initial nucleation mode peak diameter is at 23 nm (not shown on the figure). Vapour pressure data follows Nannoolal et al. (2008, A-a). Initial nucleation mode particle involatile core is 1%.*

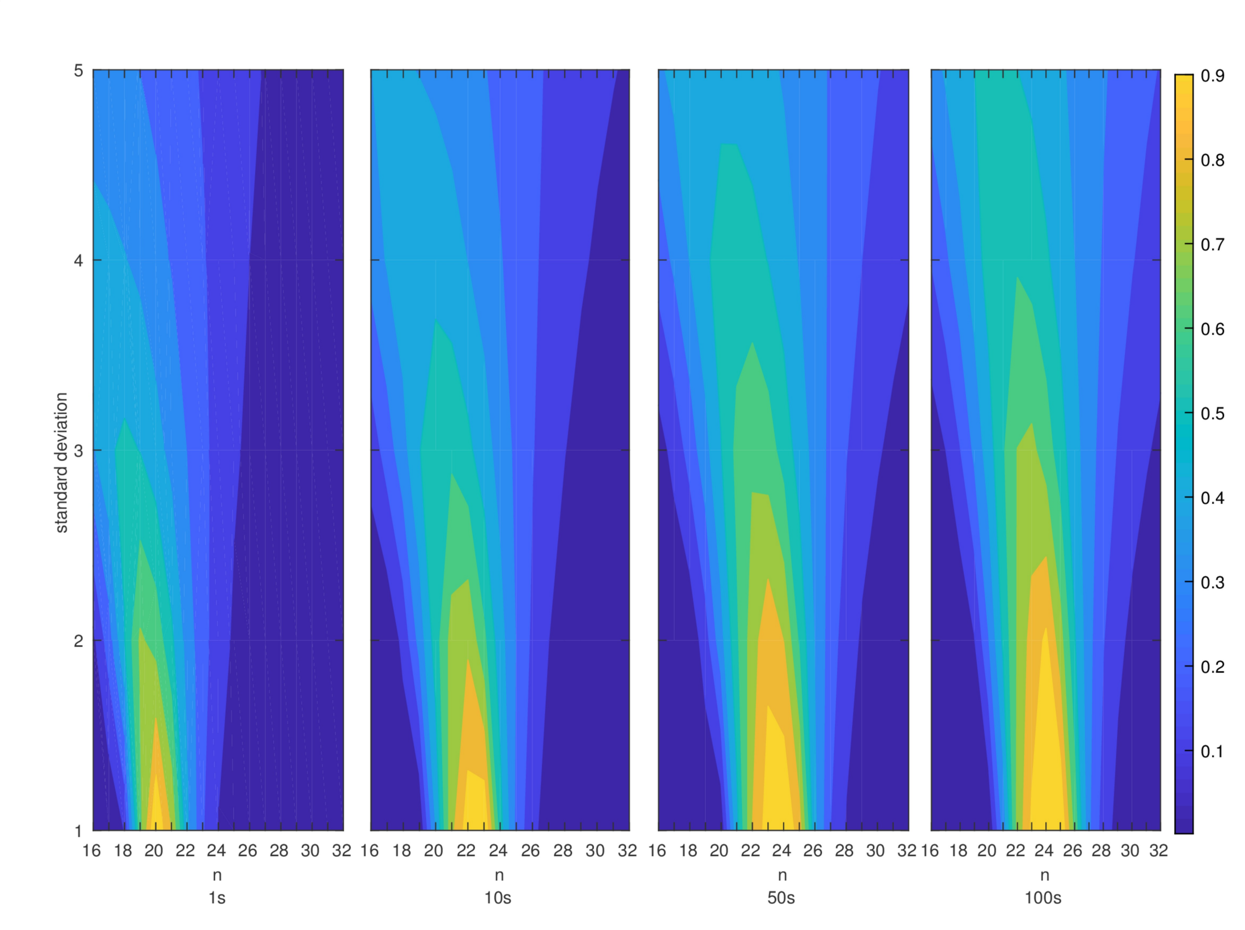

Figure 6-S. *Nucleation mode peak diameter relative difference (in %) between B-c and A-a vapour pressure parameterisations for modal compositions $C_nH_{(2n+2)}$ for n =16:32 and composition standard deviation from 1 to 5.*

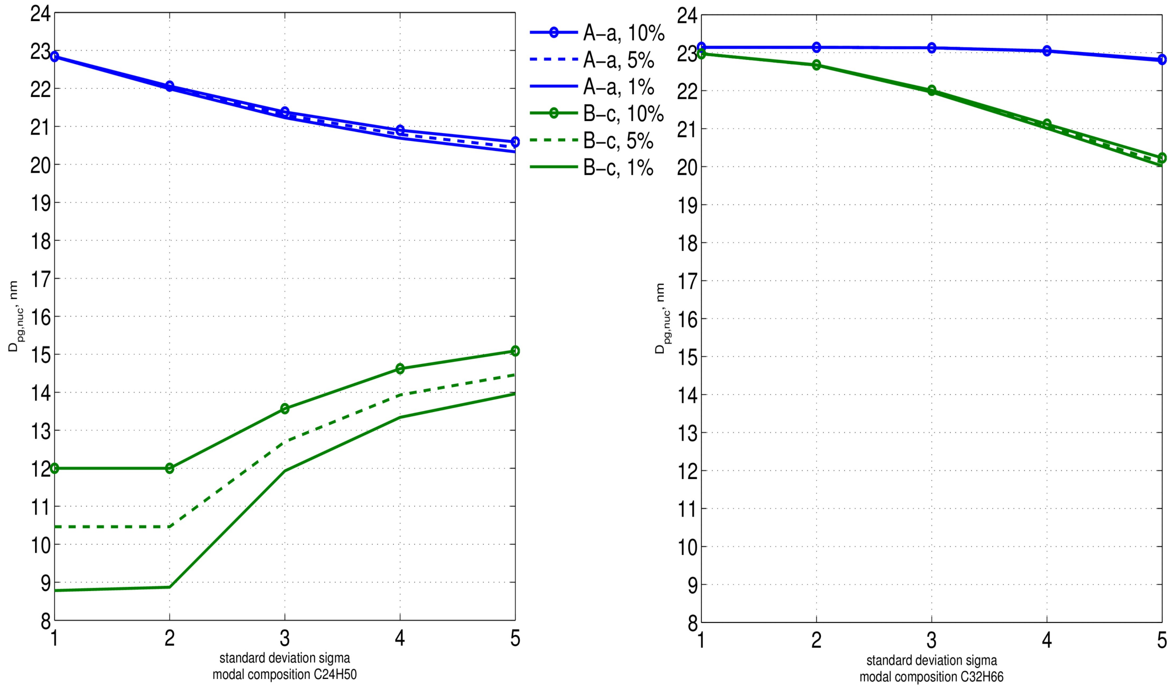

Figure 7-S. *Nucleation mode peak diameter Dp [nm] after 100s: the '100-s effective involatile core' for the nucleation mode. Results are shown at 1%, 5% and 10% initial non-volatile material in the nucleation mode particles, modal compositions* $C_{24}H_{34}$ *(left) and* $C_{32}H_{66}$ *(right) and for various composition standard deviations, sigma. Vapour pressure parameterisation follows Myrdal and Yalkowski (1997; B-c in Table 1-S) and Nannoolal et al. (2008; A-a in Table 1-S).*

σ	modal composition																
1	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	5.65E-01	2.54E-01	5.37E-02	4.39E-03	1.32E-04	1.47E-06	6.02E-09	9.04E-12	5.00E-15	1.02E-18	7.62E-23	2.10E-27	2.12E-32	7.92E-38	1.09E-43	5.82E-50	1.45E-56
	3.42E-01	4.20E-01	2.41E-01	5.35E-02	4.39E-03	1.32E-04	1.47E-06	6.02E-09	9.04E-12	5.00E-15	1.02E-18	7.62E-23	2.10E-27	2.13E-32	7.96E-38	1.15E-43	7.83E-50
	7.64E-02	2.54E-01	3.97E-01	2.40E-01	5.35E-02	4.39E-03	1.32E-04	1.47E-06	6.02E-09	9.04E-12	5.00E-15	1.02E-18	7.62E-23	2.10E-27	2.13E-32	8.41E-38	1.55E-43
	6.27E-03	5.68E-02	2.41E-01	3.95E-01	2.40E-01	5.35E-02	4.39E-03	1.32E-04	1.47E-06	6.02E-09	9.04E-12	5.00E-15	1.02E-18	7.62E-23	2.11E-27	2.26E-32	1.13E-37
	1.89E-04	4.66E-03	5.37E-02	2.40E-01	3.95E-01	2.40E-01	5.35E-02	4.39E-03	1.32E-04	1.47E-06	6.02E-09	9.04E-12	5.00E-15	1.02E-18	7.65E-23	2.23E-27	3.04E-32
	2.10E-06	1.41E-04	4.41E-03	5.35E-02	2.40E-01	3.95E-01	2.40E-01	5.35E-02	4.39E-03	1.32E-04	1.47E-06	6.02E-09	9.04E-12	5.00E-15	1.02E-18	8.09E-23	3.00E-27
	8.60E-09	1.56E-06	1.33E-04	4.39E-03	5.35E-02	2.40E-01	3.95E-01	2.40E-01	5.35E-02	4.39E-03	1.32E-04	1.47E-06	6.02E-09	9.04E-12	5.02E-15	1.08E-18	1.09E-22
	1.29E-11	6.39E-09	1.48E-06	1.33E-04	4.39E-03	5.35E-02	2.40E-01	3.95E-01	2.40E-01	5.35E-02	4.39E-03	1.32E-04	1.47E-06	6.02E-09	9.08E-12	5.31E-15	1.45E-18
	7.15E-15	9.61E-12	6.04E-09	1.47E-06	1.32E-04	4.39E-03	5.35E-02	2.40E-01	3.95E-01	2.40E-01	5.35E-02	4.39E-03	1.32E-04	1.47E-06	6.04E-09	9.61E-12	7.15E-15
	1.45E-18	5.31E-15	9.08E-12	6.02E-09	1.47E-06	1.32E-04	4.39E-03	5.35E-02	2.40E-01	3.95E-01	2.40E-01	5.35E-02	4.39E-03	1.33E-04	1.48E-06	6.39E-09	1.29E-11
	1.09E-22	1.08E-18	5.02E-15	9.04E-12	6.02E-09	1.47E-06	1.32E-04	4.39E-03	5.35E-02	2.40E-01	3.95E-01	2.40E-01	5.35E-02	4.39E-03	1.33E-04	1.56E-06	8.60E-09
	3.00E-27	8.09E-23	1.02E-18	5.00E-15	9.04E-12	6.02E-09	1.47E-06	1.32E-04	4.39E-03	5.35E-02	2.40E-01	3.95E-01	2.40E-01	5.35E-02	4.41E-03	1.41E-04	2.10E-06
	3.04E-32	2.23E-27	7.65E-23	1.02E-18	5.00E-15	9.04E-12	6.02E-09	1.47E-06	1.32E-04	4.39E-03	5.35E-02	2.40E-01	3.95E-01	2.40E-01	5.37E-02	4.66E-03	1.89E-04
	1.13E-37	2.26E-32	2.11E-27	7.62E-23	1.02E-18	5.00E-15	9.04E-12	6.02E-09	1.47E-06	1.32E-04	4.39E-03	5.35E-02	2.40E-01	3.95E-01	2.41E-01	5.68E-02	6.27E-03
	1.55E-43	8.41E-38	2.13E-32	2.10E-27	7.62E-23	1.02E-18	5.00E-15	9.04E-12	6.02E-09	1.47E-06	1.32E-04	4.39E-03	5.35E-02	2.40E-01	3.97E-01	2.54E-01	7.64E-02
	7.83E-50	1.15E-43	7.96E-38	2.13E-32	2.10E-27	7.62E-23	1.02E-18	5.00E-15	9.04E-12	6.02E-09	1.47E-06	1.32E-04	4.39E-03	5.35E-02	2.41E-01	4.20E-01	3.42E-01
	1.45E-56	5.82E-50	1.09E-43	7.92E-38	2.12E-32	2.10E-27	7.62E-23	1.02E-18	5.00E-15	9.04E-12	6.02E-09	1.47E-06	1.32E-04	4.39E-03	5.37E-02	2.54E-01	5.65E-01
	9.90E-001																
2	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	3.29E-01	2.25E-01	1.34E-01	6.67E-02	2.70E-02	8.70E-03	2.19E-03	4.32E-04	6.62E-05	7.91E-06	7.36E-07	5.35E-08	3.04E-09	1.37E-10	5.04E-12	1.55E-13	4.17E-15
	2.91E-01	2.55E-01	1.94E-01	1.25E-01	6.49E-02	2.68E-02	8.68E-03	2.19E-03	4.32E-04	6.63E-05	7.92E-06	7.38E-07	5.39E-08	3.13E-09	1.47E-10	5.83E-12	2.01E-13
	2.00E-01	2.25E-01	2.20E-01	1.81E-01	1.21E-01	6.43E-02	2.67E-02	8.68E-03	2.19E-03	4.32E-04	6.63E-05	7.93E-06	7.44E-07	5.54E-08	3.35E-09	1.70E-10	7.54E-12
	1.07E-01	1.54E-01	1.94E-01	2.05E-01	1.76E-01	1.20E-01	6.41E-02	2.67E-02	8.68E-03	2.19E-03	4.32E-04	6.64E-05	8.00E-06	7.65E-07	5.94E-08	3.88E-09	2.20E-10
	4.46E-02	8.26E-02	1.34E-01	1.81E-01	2.00E-01	1.75E-01	1.20E-01	6.41E-02	2.67E-02	8.68E-03	2.19E-03	4.33E-04	6.70E-05	8.23E-06	8.21E-07	6.87E-08	5.01E-09
	1.45E-02	3.45E-02	7.15E-02	1.25E-01	1.76E-01	1.98E-01	1.74E-01	1.20E-01	6.41E-02	2.67E-02	8.68E-03	2.20E-03	4.37E-04	6.89E-05	8.82E-06	9.49E-07	8.89E-08
	3.66E-03	1.12E-02	2.98E-02	6.67E-02	1.21E-01	1.75E-01	1.98E-01	1.74E-01	1.20E-01	6.41E-02	2.67E-02	8.70E-03	2.22E-03	4.49E-04	7.39E-05	1.02E-05	1.23E-06
	7.20E-04	2.83E-03	9.68E-03	2.78E-02	6.49E-02	1.20E-01	1.74E-01	1.97E-01	1.74E-01	1.20E-01	6.41E-02	2.68E-02	8.78E-03	2.28E-03	4.82E-04	8.54E-05	1.32E-05
	1.10E-04	5.57E-04	2.45E-03	9.02E-03	2.70E-02	6.43E-02	1.20E-01	1.74E-01	1.97E-01	1.74E-01	1.20E-01	6.43E-02	2.70E-02	9.02E-03	2.45E-03	5.57E-04	1.10E-04
	1.32E-05	8.54E-05	4.82E-04	2.28E-03	8.78E-03	2.68E-02	6.41E-02	1.20E-01	1.74E-01	1.97E-01	1.74E-01	1.20E-01	6.49E-02	2.78E-02	9.68E-03	2.83E-03	7.20E-04
	1.23E-06	1.02E-05	7.39E-05	4.49E-04	2.22E-03	8.70E-03	2.67E-02	6.41E-02	1.20E-01	1.74E-01	1.98E-01	1.75E-01	1.21E-01	6.67E-02	2.98E-02	1.12E-02	3.66E-03
	8.89E-08	9.49E-07	8.82E-06	6.89E-05	4.37E-04	2.20E-03	8.68E-03	2.67E-02	6.41E-02	1.20E-01	1.74E-01	1.98E-01	1.76E-01	1.25E-01	7.15E-02	3.45E-02	1.45E-02
	5.01E-09	6.87E-08	8.21E-07	8.23E-06	6.70E-05	4.33E-04	2.19E-03	8.68E-03	2.67E-02	6.41E-02	1.20E-01	1.75E-01	2.00E-01	1.81E-01	1.34E-01	8.26E-02	4.46E-02
	2.20E-10	3.88E-09	5.94E-08	7.65E-07	8.00E-06	6.64E-05	4.32E-04	2.19E-03	8.68E-03	2.67E-02	6.41E-02	1.20E-01	1.76E-01	2.05E-01	1.94E-01	1.54E-01	1.07E-01
	7.54E-12	1.70E-10	3.35E-09	5.54E-08	7.44E-07	7.93E-06	6.63E-05	4.32E-04	2.19E-03	8.68E-03	2.67E-02	6.43E-02	1.21E-01	1.81E-01	2.20E-01	2.25E-01	2.00E-01
	2.01E-13	5.83E-12	1.47E-10	3.13E-09	5.39E-08	7.38E-07	7.92E-06	6.63E-05	4.32E-04	2.19E-03	8.68E-03	2.68E-02	6.49E-02	1.25E-01	1.94E-01	2.55E-01	2.91E-01
	4.17E-15	1.55E-13	5.04E-12	1.37E-10	3.04E-09	5.35E-08	7.36E-07	7.91E-06	6.62E-05	4.32E-04	2.19E-03	8.70E-03	2.70E-02	6.67E-02	1.34E-01	2.25E-01	3.29E-01
3	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	2.32E-01	1.80E-01	1.32E-01	9.08E-02	5.79E-02	3.39E-02	1.81E-02	8.71E-03	3.78E-03	1.47E-03	5.17E-04	1.64E-04	4.73E-05	1.25E-05	3.08E-06	7.09E-07	1.55E-07
	2.20E-01	1.90E-01	1.56E-01	1.20E-01	8.55E-02	5.60E-02	3.33E-02	1.79E-02	8.69E-03	3.79E-03	1.48E-03	5.26E-04	1.70E-04	5.02E-05	1.38E-05	3.55E-06	8.66E-07
	1.86E-01	1.80E-01	1.65E-01	1.42E-01	1.13E-01	8.26E-02	5.49E-02	3.31E-02	1.79E-02	8.71E-03	3.82E-03	1.51E-03	5.45E-04	1.80E-04	5.53E-05	1.59E-05	4.34E-06
	1.41E-01	1.52E-01	1.56E-01	1.50E-01	1.33E-01	1.09E-01	8.11E-02	5.45E-02	3.30E-02	1.79E-02	8.78E-03	3.89E-03	1.57E-03	5.79E-04	1.98E-04	6.38E-05	1.94E-05
	9.55E-02	1.15E-01	1.32E-01	1.42E-01	1.41E-01	1.29E-01	1.07E-01	8.04E-02	5.44E-02	3.31E-02	1.81E-02	8.95E-03	4.03E-03	1.66E-03	6.37E-04	2.29E-04	7.80E-05
	5.79E-02	7.82E-02	1.00E-01	1.20E-01	1.33E-01	1.36E-01	1.26E-01	1.06E-01	8.02E-02	5.45E-02	3.33E-02	1.84E-02	9.26E-03	4.28E-03	1.83E-03	7.35E-04	2.80E-04
	3.15E-02	4.74E-02	6.78E-02	9.08E-02	1.13E-01	1.29E-01	1.34E-01	1.25E-01	1.06E-01	8.04E-02	5.49E-02	3.39E-02	1.91E-02	9.84E-03	4.71E-03	2.11E-03	8.98E-04
	1.53E-02	2.57E-02	4.11E-02	6.15E-02	8.55E-02	1.09E-01	1.26E-01	1.33E-01	1.25E-01	1.06E-01	8.11E-02	5.60E-02	3.51E-02	2.03E-02	1.08E-02	5.43E-03	2.58E-03
	6.64E-03	1.25E-02	2.23E-02	3.73E-02	5.79E-02	8.26E-02	1.07E-01	1.25E-01	1.32E-01	1.25E-01	1.07E-01	8.26E-02	5.79E-02	3.73E-02	2.23E-02	1.25E-02	6.64E-03
	2.58E-03	5.43E-03	1.08E-02	2.03E-02	3.51E-02	5.60E-02	8.11E-02	1.06E-01	1.25E-01	1.33E-01	1.26E-01	1.09E-01	8.55E-02	6.15E-02	4.11E-02	2.57E-02	1.53E-02
	8.98E-04	2.11E-03	4.71E-03	9.84E-03	1.91E-02	3.39E-02	5.49E-02	8.04E-02	1.06E-01	1.25E-01	1.34E-01	1.29E-01	1.13E-01	9.08E-02	6.78E-02	4.74E-02	3.15E-02
	2.80E-04	7.35E-04	1.83E-03	4.28E-03	9.26E-03	1.84E-02	3.33E-02	5.45E-02	8.02E-02	1.06E-01	1.26E-01	1.36E-01	1.33E-01	1.20E-01	1.00E-01	7.82E-02	5.79E-02
	7.80E-05	2.29E-04	6.37E-04	1.66E-03	4.03E-03	8.95E-03	1.81E-02	3.31E-02	5.44E-02	8.04E-02	1.07E-01	1.29E-01	1.41E-01	1.42E-01	1.32E-01	1.15E-01	9.55E-02
	1.94E-05	6.38E-05	1.98E-04	5.79E-04	1.57E-03	3.89E-03	8.78E-03	1.79E-02	3.30E-02	5.45E-02	8.11E-02	1.09E-01	1.33E-01	1.50E-01	1.56E-01	1.52E-01	1.41E-01
	4.34E-06	1.59E-05	5.53E-05	1.80E-04	5.45E-04	1.51E-03	3.82E-03	8.71E-03	1.79E-02	3.31E-02	5.49E-02	8.26E-02	1.13E-01	1.42E-01	1.65E-01	1.80E-01	1.86E-01
	8.66E-07	3.55E-06	1.38E-05	5.02E-05	1.70E-04	5.26E-04	1.48E-03	3.79E-03	8.69E-03	1.79E-02	3.33E-02	5.60E-02	8.55E-02	1.20E-01	1.56E-01	1.90E-01	2.20E-01
	1.55E-07	7.09E-07	3.08E-06	1.25E-05	4.73E-05	1.64E-04	5.17E-04	1.47E-03	3.78E-03	8.71E-03	1.81E-02	3.39E-02	5.79E-02	9.08E-02	1.32E-01	1.80E-01	2.32E-01
4	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	1.80E-01	1.48E-01	1.19E-01	9.21E-02	6.89E-02	4.95E-02	3.40E-02	2.22E-02	1.38E-02	8.17E-03	4.60E-03	2.46E-03	1.26E-03	6.20E-04	2.94E-04	1.35E-04	6.02E-05
	1.74E-01	1.53E-01	1.30E-01	1.08E-01	8.57E-02	6.55E-02	4.79E-02	3.33E-02	2.21E-02	1.39E-02	8.32E-03	4.75E-03	2.59E-03	1.36E-03	6.84E-04	3.34E-04	1.59E-04
	1.58E-01	1.48E-01	1.34E-01	1.18E-01	1.00E-01	8.15E-02	6.34E-02	4.70E-02	3.32E-02	2.22E-02	1.42E-02	8.59E-03	4.99E-03	2.78E-03	1.49E-03	7.77E-04	3.93E-04
	1.36E-01	1.35E-01	1.30E-01	1.22E-01	1.10E-01	9.53E-02	7.89E-02	6.23E-02	4.68E-02	3.33E-02	2.26E-02	1.46E-02	9.03E-03	5.36E-03	3.06E-03	1.70E-03	9.13E-04
	1.09E-01	1.15E-01	1.19E-01	1.18E-01	1.14E-01	1.05E-01	9.23E-02	7.75E-02	6.19E-02	4.70E-02	3.40E-02	2.34E-02	1.54E-02	9.70E-03	5.91E-03	3.48E-03	1.99E-03
	8.22E-02	9.26E-02	1.01E-01	1.08E-01	1.10E-01	1.08E-01	1.01E-01	9.06E-02	7.71E-02	6.23E-02	4.79E-02	3.51E-02	2.46E-02	1.65E-02	1.07E-02	6.71E-03	4.09E-03
	5.83E-02	6.99E-02	8.15E-02	9.21E-02	1.00E-01	1.05E-01	1.05E-01	9.96E-02	9.01E-02	7.75E-02	6.34E-02	4.95E-02	3.69E-02	2.64E-02	1.82E-02	1.22E-02	7.89E-03
	3.88E-02	4.96E-02	6.16E-02	7.40E-02	8.57E-02	9.53E-02	1.01E-01	1.03E-01	9.90E-02	9.06E-02	7.89E-02	6.55E-02	5.20E-02	3.96E-02	2.91E-02	2.07E-02	1.43E-02
	2.43E-02	3.30E-02	4.36E-02	5.58E-02	6.89E-02	8.15E-02	9.23E-02	9.96E-02	1.02E-01	9.96E-02	9.23E-02	8.15E-02	6.89E-02	5.58E-02	4.36E-02	3.30E-02	2.43E-02
	1.43E-02	2.07E-02	2.91E-02	3.96E-02	5.20E-02	6.55E-02	7.89E-02	9.06E-02	9.90E-02	1.03E-01	1.01E-01	9.53E-02	8.57E-02	7.40E-02	6.16E-02	4.96E-02	3.88E-02
	7.89E-03	1.22E-02	1.82E-02	2.64E-02	3.69E-02	4.95E-02	6.34E-02	7.75E-02	9.01E-02	9.96E-02	1.05E-01	1.05E-01	1.00E-01	9.21E-02	8.15E-02	6.99E-02	5.83E-02
	4.09E-03	6.71E-03	1.07E-02	1.65E-02	2.46E-02	3.51E-02	4.79E-02	6.23E-02	7.71E-02	9.06E-02	1.01E-01	1.08E-01	1.10E-01	1.08E-01	1.01E-01	9.26E-02	8.22E-02
	1.99E-03	3.48E-03	5.91E-03	9.70E-03	1.54E-02	2.34E-02	3.40E-02	4.70E-02	6.19E-02	7.75E-02	9.23E-02	1.05E-01	1.14E-01	1.18E-01	1.19E-01	1.15E-01	1.09E-01
	9.13E-04	1.70E-03	3.06E-03	5.36E-03	9.03E-03	1.46E-02	2.26E-02	3.33E-02	4.68E-02	6.23E-02	7.89E-02	9.53E-02	1.10E-01	1.22E-01	1.30E-01	1.35E-01	1.36E-01
	3.93E-04	7.77E-04	1.49E-03	2.78E-03	4.99E-03	8.59E-03	1.42E-02	2.22E-02	3.32E-02	4.70E-02	6.34E-02	8.15E-02	1.00E-01	1.18E-01	1.34E-01	1.48E-01	1.58E-01
	1.59E-04	3.34E-04	6.84E-04	1.36E-03	2.59E-03	4.75E-03	8.32E-03	1.39E-02	2.21E-02	3.33E-02	4.79E-02	6.55E-02	8.57E-02	1.08E-01	1.30E-01	1.53E-01	1.74E-01
	6.02E-05	1.35E-04	2.94E-04	6.20E-04	1.26E-03	2.46E-03	4.60E-03	8.17E-03	1.38E-02	2.22E-02	3.40E-02	4.95E-02	6.89E-02	9.21E-02	1.19E-01	1.48E-01	1.80E-01
5	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	1.46E-01	1.25E-01	1.06E-01	8.74E-02	7.08E-02	5.61E-02	4.34E-02	3.28E-02	2.41E-02	1.73E-02	1.21E-02	8.22E-03	5.47E-03	3.56E-03	2.27E-03	1.42E-03	8.75E-04
	1.44E-01	1.28E-01	1.12E-01	9.66E-02	8.14E-02	6.72E-02	5.41E-02	4.25E-02	3.25E-02	2.43E-02	1.76E-02	1.25E-02	8.67E-03	5.87E-03	3.90E-03	2.54E-03	1.63E-03
	1.35E-01	1.25E-01	1.14E-01	1.03E-01	9.00E-02	7.72E-02	6.47E-02	5.29E-02	4.22E-02	3.28E-02	2.48E-02	1.83E-02	1.32E-02	9.30E-03	6.43E-03	4.36E-03	2.91E-03
	1.22E-01	1.18E-01	1.12E-01	1.05E-01	9.56E-02	8.54E-02	7.45E-02	6.34E-02	5.26E-02	4.25E-02	3.35E-02	2.57E-02	1.93E-02	1.42E-02	1.02E-02	7.18E-03	4.99E-03
	1.06E-01	1.07E-01	1.06E-01	1.03E-01	9.75E-02	9.07E-02	8.23E-02	7.29E-02	6.29E-02	5.29E-02	4.34E-02	3.47E-02	2.71E-02	2.07E-02	1.55E-02	1.14E-02	8.22E-03
	8.88E-02	9.29E-02	9.56E-02	9.66E-02	9.56E-02	9.25E-02	8.74E-02	8.06E-02	7.24E-02	6.34E-02	5.41E-02	4.50E-02	3.66E-02	2.91E-02	2.27E-02	1.73E-02	1.30E-02
	7.13E-02	7.76E-02	8.31E-02	8.74E-02	9.00E-02	9.07E-02	8.92E-02	8.56E-02	8.00E-02	7.29E-02	6.47E-02	5.61E-02	4.75E-02	3.93E-02	3.18E-02	2.53E-02	1.98E-02
	5.50E-02	6.23E-02	6.94E-02	7.60E-02	8.14E-02	8.54E-02	8.74E-02	8.73E-02	8.50E-02	8.06E-02	7.45E-02	6.72E-02	5.91E-02	5.09E-02	4.30E-02	3.56E-02	2.90E-02
	4.07E-02	4.80E-02	5.57E-02	6.35E-02	7.08E-02	7.72E-02	8.23E-02	8.56E-02	8.67E-02	8.56E-02	8.23E-02	7.72E-02	7.08E-02	6.35E-02	5.57E-02	4.80E-02	4.07E-02
	2.90E-02	3.56E-02	4.30E-02	5.09E-02	5.91E-02	6.72E-02	7.45E-02	8.06E-02	8.50E-02	8.73E-02	8.74E-02	8.54E-02	8.14E-02	7.60E-02	6.94E-02	6.23E-02	5.50E-02
	1.98E-02	2.53E-02	3.18E-02	3.93E-02	4.75E-02	5.61E-02	6.47E-02	7.29E-02	8.00E-02	8.56E-02	8.92E-02	9.07E-02	9.00E-02	8.74E-02	8.31E-02	7.76E-02	7.13E-02
	1.30E-02	1.73E-02	2.27E-02	2.91E-02	3.66E-02	4.50E-02	5.41E-02	6.34E-02	7.24E-02	8.06E-02	8.74E-02	9.25E-02	9.56E-02	9.66E-02	9.56E-02	9.29E-02	8.88E-02
	8.22E-03	1.14E-02	1.55E-02	2.07E-02	2.71E-02	3.47E-02	4.34E-02	5.29E-02	6.29E-02	7.29E-02	8.23E-02	9.07E-02	9.75E-02	1.03E-01	1.06E-01	1.07E-01	1.06E-01
	4.99E-03	7.18E-03	1.02E-02	1.42E-02	1.93E-02	2.57E-02	3.35E-02	4.25E-02	5.26E-02	6.34E-02	7.45E-02	8.54E-02	9.56E-02	1.05E-01	1.12E-01	1.18E-01	1.22E-01
	2.91E-03	4.36E-03	6.43E-03	9.30E-03	1.32E-02	1.83E-02	2.48E-02	3.28E-02	4.22E-02	5.29E-02	6.47E-02	7.72E-02	9.00E-02	1.03E-01	1.14E-01	1.25E-01	1.35E-01
	1.63E-03	2.54E-03	3.90E-03	5.87E-03	8.67E-03	1.25E-02	1.76E-02	2.43E-02	3.25E-02	4.25E-02	5.41E-02	6.72E-02	8.14E-02	9.66E-02	1.12E-01	1.28E-01	1.44E-01
	8.75E-04	1.42E-03	2.27E-03	3.56E-03	5.47E-03	8.22E-03	1.21E-02	1.73E-02	2.41E-02	3.28E-02	4.34E-02	5.61E-02	7.08E-02	8.74E-02	1.06E-01	1.25E-01	1.46E-01

Table 1-S. *Input modal composition mass fractions (by columns) in the nucleation mode and composition standard deviation for involatile core of 1%.*

σ	modal composition																
1	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	5.42E-01	2.44E-01	5.15E-02	4.21E-03	1.27E-04	1.41E-06	5.77E-09	8.68E-12	4.80E-15	9.77E-19	7.31E-23	2.01E-27	2.04E-32	7.60E-38	1.05E-43	5.58E-50	1.39E-56
	3.29E-01	4.03E-01	2.31E-01	5.13E-02	4.21E-03	1.27E-04	1.41E-06	5.77E-09	8.68E-12	4.80E-15	9.77E-19	7.31E-23	2.01E-27	2.04E-32	7.63E-38	1.11E-43	7.51E-50
	7.33E-02	2.44E-01	3.81E-01	2.30E-01	5.13E-02	4.21E-03	1.27E-04	1.41E-06	5.77E-09	8.68E-12	4.80E-15	9.77E-19	7.31E-23	2.01E-27	2.05E-32	8.07E-38	1.49E-43
	6.02E-03	5.45E-02	2.31E-01	3.79E-01	2.30E-01	5.13E-02	4.21E-03	1.27E-04	1.41E-06	5.77E-09	8.68E-12	4.80E-15	9.77E-19	7.31E-23	2.02E-27	2.17E-32	1.09E-37
	1.82E-04	4.47E-03	5.15E-02	2.30E-01	3.79E-01	2.30E-01	5.13E-02	4.21E-03	1.27E-04	1.41E-06	5.77E-09	8.68E-12	4.80E-15	9.77E-19	7.34E-23	2.14E-27	2.92E-32
	2.02E-06	1.35E-04	4.23E-03	5.13E-02	2.30E-01	3.79E-01	2.30E-01	5.13E-02	4.21E-03	1.27E-04	1.41E-06	5.77E-09	8.68E-12	4.80E-15	9.81E-19	7.76E-23	2.88E-27
	8.25E-09	1.50E-06	1.28E-04	4.21E-03	5.13E-02	2.30E-01	3.79E-01	2.30E-01	5.13E-02	4.21E-03	1.27E-04	1.41E-06	5.77E-09	8.68E-12	4.82E-15	1.04E-18	1.05E-22
	1.24E-11	6.13E-09	1.42E-06	1.27E-04	4.21E-03	5.13E-02	2.30E-01	3.79E-01	2.30E-01	5.13E-02	4.21E-03	1.27E-04	1.41E-06	5.77E-09	8.72E-12	5.10E-15	1.40E-18
	6.86E-15	9.22E-12	5.80E-09	1.41E-06	1.27E-04	4.21E-03	5.13E-02	2.30E-01	3.79E-01	2.30E-01	5.13E-02	4.21E-03	1.27E-04	1.41E-06	5.80E-09	9.22E-12	6.86E-15
	1.40E-18	5.10E-15	8.72E-12	5.77E-09	1.41E-06	1.27E-04	4.21E-03	5.13E-02	2.30E-01	3.79E-01	2.30E-01	5.13E-02	4.21E-03	1.27E-04	1.42E-06	6.13E-09	1.24E-11
	1.05E-22	1.04E-18	4.82E-15	8.68E-12	5.77E-09	1.41E-06	1.27E-04	4.21E-03	5.13E-02	2.30E-01	3.79E-01	2.30E-01	5.13E-02	4.21E-03	1.28E-04	1.50E-06	8.25E-09
	2.88E-27	7.76E-23	9.81E-19	4.80E-15	8.68E-12	5.77E-09	1.41E-06	1.27E-04	4.21E-03	5.13E-02	2.30E-01	3.79E-01	2.30E-01	5.13E-02	4.23E-03	1.35E-04	2.02E-06
	2.92E-32	2.14E-27	7.34E-23	9.77E-19	4.80E-15	8.68E-12	5.77E-09	1.41E-06	1.27E-04	4.21E-03	5.13E-02	2.30E-01	3.79E-01	2.30E-01	5.15E-02	4.47E-03	1.82E-04
	1.09E-37	2.17E-32	2.02E-27	7.31E-23	9.77E-19	4.80E-15	8.68E-12	5.77E-09	1.41E-06	1.27E-04	4.21E-03	5.13E-02	2.30E-01	3.79E-01	2.31E-01	5.45E-02	6.02E-03
	1.49E-43	8.07E-38	2.05E-32	2.01E-27	7.31E-23	9.77E-19	4.80E-15	8.68E-12	5.77E-09	1.41E-06	1.27E-04	4.21E-03	5.13E-02	2.30E-01	3.81E-01	2.44E-01	7.33E-02
	7.51E-50	1.11E-43	7.63E-38	2.04E-32	2.01E-27	7.31E-23	9.77E-19	4.80E-15	8.68E-12	5.77E-09	1.41E-06	1.27E-04	4.21E-03	5.13E-02	2.31E-01	4.03E-01	3.29E-01
	1.39E-56	5.58E-50	1.05E-43	7.60E-38	2.04E-32	2.01E-27	7.31E-23	9.77E-19	4.80E-15	8.68E-12	5.77E-09	1.41E-06	1.27E-04	4.21E-03	5.15E-02	2.44E-01	5.42E-01
	9.50E-001																
2	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	3.16E-01	2.16E-01	1.28E-01	6.40E-02	2.59E-02	8.35E-03	2.11E-03	4.15E-04	6.36E-05	7.59E-06	7.07E-07	5.13E-08	2.92E-09	1.32E-10	4.84E-12	1.49E-13	4.00E-15
	2.79E-01	2.44E-01	1.86E-01	1.20E-01	6.22E-02	2.57E-02	8.33E-03	2.11E-03	4.15E-04	6.36E-05	7.60E-06	7.08E-07	5.18E-08	3.00E-09	1.41E-10	5.59E-12	1.93E-13
	1.92E-01	2.16E-01	2.11E-01	1.74E-01	1.16E-01	6.17E-02	2.57E-02	8.33E-03	2.11E-03	4.15E-04	6.36E-05	7.61E-06	7.14E-07	5.32E-08	3.22E-09	1.63E-10	7.23E-12
	1.03E-01	1.48E-01	1.86E-01	1.97E-01	1.69E-01	1.15E-01	6.16E-02	2.56E-02	8.33E-03	2.11E-03	4.15E-04	6.37E-05	7.68E-06	7.34E-07	5.70E-08	3.72E-09	2.11E-10
	4.28E-02	7.93E-02	1.28E-01	1.74E-01	1.92E-01	1.68E-01	1.15E-01	6.15E-02	2.56E-02	8.33E-03	2.11E-03	4.16E-04	6.43E-05	7.90E-06	7.87E-07	6.59E-08	4.81E-09
	1.39E-02	3.31E-02	6.86E-02	1.20E-01	1.69E-01	1.90E-01	1.67E-01	1.15E-01	6.15E-02	2.56E-02	8.33E-03	2.11E-03	4.19E-04	6.61E-05	8.47E-06	9.10E-07	8.53E-08
	3.51E-03	1.07E-02	2.86E-02	6.40E-02	1.16E-01	1.68E-01	1.90E-01	1.67E-01	1.15E-01	6.15E-02	2.57E-02	8.35E-03	2.13E-03	4.31E-04	7.09E-05	9.79E-06	1.18E-06
	6.91E-04	2.71E-03	9.28E-03	2.67E-02	6.22E-02	1.15E-01	1.67E-01	1.90E-01	1.67E-01	1.15E-01	6.16E-02	2.57E-02	8.42E-03	2.19E-03	4.62E-04	8.19E-05	1.27E-05
	1.06E-04	5.34E-04	2.35E-03	8.66E-03	2.59E-02	6.17E-02	1.15E-01	1.67E-01	1.90E-01	1.67E-01	1.15E-01	6.17E-02	2.59E-02	8.66E-03	2.35E-03	5.34E-04	1.06E-04
	1.27E-05	8.19E-05	4.62E-04	2.19E-03	8.42E-03	2.57E-02	6.16E-02	1.15E-01	1.67E-01	1.90E-01	1.67E-01	1.15E-01	6.22E-02	2.67E-02	9.28E-03	2.71E-03	6.91E-04
	1.18E-06	9.79E-06	7.09E-05	4.31E-04	2.13E-03	8.35E-03	2.57E-02	6.15E-02	1.15E-01	1.67E-01	1.90E-01	1.68E-01	1.16E-01	6.40E-02	2.86E-02	1.07E-02	3.51E-03
	8.53E-08	9.10E-07	8.47E-06	6.61E-05	4.19E-04	2.11E-03	8.33E-03	2.56E-02	6.15E-02	1.15E-01	1.67E-01	1.90E-01	1.69E-01	1.20E-01	6.86E-02	3.31E-02	1.39E-02
	4.81E-09	6.59E-08	7.87E-07	7.90E-06	6.43E-05	4.16E-04	2.11E-03	8.33E-03	2.56E-02	6.15E-02	1.15E-01	1.68E-01	1.92E-01	1.74E-01	1.28E-01	7.93E-02	4.28E-02
	2.11E-10	3.72E-09	5.70E-08	7.34E-07	7.68E-06	6.37E-05	4.15E-04	2.11E-03	8.33E-03	2.56E-02	6.16E-02	1.15E-01	1.69E-01	1.97E-01	1.86E-01	1.48E-01	1.03E-01
	7.23E-12	1.63E-10	3.22E-09	5.32E-08	7.14E-07	7.61E-06	6.36E-05	4.15E-04	2.11E-03	8.33E-03	2.57E-02	6.17E-02	1.16E-01	1.74E-01	2.11E-01	2.16E-01	1.92E-01
	1.93E-13	5.59E-12	1.41E-10	3.00E-09	5.18E-08	7.08E-07	7.60E-06	6.36E-05	4.15E-04	2.11E-03	8.33E-03	2.57E-02	6.22E-02	1.20E-01	1.86E-01	2.44E-01	2.79E-01
	4.00E-15	1.49E-13	4.84E-12	1.32E-10	2.92E-09	5.13E-08	7.07E-07	7.59E-06	6.36E-05	4.15E-04	2.11E-03	8.35E-03	2.59E-02	6.40E-02	1.28E-01	2.16E-01	3.16E-01
3	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	2.23E-01	1.73E-01	1.27E-01	8.71E-02	5.56E-02	3.26E-02	1.74E-02	8.36E-03	3.62E-03	1.41E-03	4.96E-04	1.57E-04	4.54E-05	1.20E-05	2.95E-06	6.80E-07	1.48E-07
	2.11E-01	1.82E-01	1.50E-01	1.15E-01	8.20E-02	5.37E-02	3.20E-02	1.72E-02	8.34E-03	3.63E-03	1.42E-03	5.05E-04	1.63E-04	4.82E-05	1.32E-05	3.41E-06	8.31E-07
	1.79E-01	1.73E-01	1.58E-01	1.36E-01	1.08E-01	7.92E-02	5.27E-02	3.17E-02	1.72E-02	8.36E-03	3.66E-03	1.45E-03	5.23E-04	1.73E-04	5.31E-05	1.53E-05	4.16E-06
	1.35E-01	1.46E-01	1.50E-01	1.44E-01	1.28E-01	1.05E-01	7.78E-02	5.23E-02	3.16E-02	1.72E-02	8.43E-03	3.73E-03	1.50E-03	5.55E-04	1.90E-04	6.12E-05	1.87E-05
	9.17E-02	1.11E-01	1.27E-01	1.36E-01	1.35E-01	1.24E-01	1.03E-01	7.71E-02	5.22E-02	3.17E-02	1.74E-02	8.59E-03	3.86E-03	1.60E-03	6.11E-04	2.20E-04	7.48E-05
	5.56E-02	7.50E-02	9.59E-02	1.15E-01	1.28E-01	1.31E-01	1.21E-01	1.02E-01	7.70E-02	5.23E-02	3.20E-02	1.77E-02	8.89E-03	4.10E-03	1.76E-03	7.05E-04	2.68E-04
	3.02E-02	4.55E-02	6.50E-02	8.71E-02	1.08E-01	1.24E-01	1.28E-01	1.20E-01	1.02E-01	7.71E-02	5.27E-02	3.26E-02	1.83E-02	9.44E-03	4.52E-03	2.03E-03	8.62E-04
	1.47E-02	2.47E-02	3.94E-02	5.91E-02	8.20E-02	1.05E-01	1.21E-01	1.27E-01	1.20E-01	1.02E-01	7.78E-02	5.37E-02	3.37E-02	1.94E-02	1.04E-02	5.21E-03	2.48E-03
	6.37E-03	1.20E-02	2.14E-02	3.58E-02	5.56E-02	7.92E-02	1.03E-01	1.20E-01	1.27E-01	1.20E-01	1.03E-01	7.92E-02	5.56E-02	3.58E-02	2.14E-02	1.20E-02	6.37E-03
	2.48E-03	5.21E-03	1.04E-02	1.94E-02	3.37E-02	5.37E-02	7.78E-02	1.02E-01	1.20E-01	1.27E-01	1.21E-01	1.05E-01	8.20E-02	5.91E-02	3.94E-02	2.47E-02	1.47E-02
	8.62E-04	2.03E-03	4.52E-03	9.44E-03	1.83E-02	3.26E-02	5.27E-02	7.71E-02	1.02E-01	1.20E-01	1.28E-01	1.24E-01	1.08E-01	8.71E-02	6.50E-02	4.55E-02	3.02E-02
	2.68E-04	7.05E-04	1.76E-03	4.10E-03	8.89E-03	1.77E-02	3.20E-02	5.23E-02	7.70E-02	1.02E-01	1.21E-01	1.31E-01	1.28E-01	1.15E-01	9.59E-02	7.50E-02	5.56E-02
	7.48E-05	2.20E-04	6.11E-04	1.60E-03	3.86E-03	8.59E-03	1.74E-02	3.17E-02	5.22E-02	7.71E-02	1.03E-01	1.24E-01	1.35E-01	1.36E-01	1.27E-01	1.11E-01	9.17E-02
	1.87E-05	6.12E-05	1.90E-04	5.55E-04	1.50E-03	3.73E-03	8.43E-03	1.72E-02	3.16E-02	5.23E-02	7.78E-02	1.05E-01	1.28E-01	1.44E-01	1.50E-01	1.46E-01	1.35E-01
	4.16E-06	1.53E-05	5.31E-05	1.73E-04	5.23E-04	1.45E-03	3.66E-03	8.36E-03	1.72E-02	3.17E-02	5.27E-02	7.92E-02	1.08E-01	1.36E-01	1.58E-01	1.73E-01	1.79E-01
	8.31E-07	3.41E-06	1.32E-05	4.82E-05	1.63E-04	5.05E-04	1.42E-03	3.63E-03	8.34E-03	1.72E-02	3.20E-02	5.37E-02	8.20E-02	1.15E-01	1.50E-01	1.82E-01	2.11E-01
	1.48E-07	6.80E-07	2.95E-06	1.20E-05	4.54E-05	1.57E-04	4.96E-04	1.41E-03	3.62E-03	8.36E-03	1.74E-02	3.26E-02	5.56E-02	8.71E-02	1.27E-01	1.73E-01	2.23E-01
4	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	1.72E-01	1.42E-01	1.14E-01	8.84E-02	6.61E-02	4.75E-02	3.26E-02	2.13E-02	1.33E-02	7.84E-03	4.41E-03	2.36E-03	1.21E-03	5.95E-04	2.82E-04	1.30E-04	5.78E-05
	1.67E-01	1.47E-01	1.25E-01	1.03E-01	8.23E-02	6.29E-02	4.59E-02	3.20E-02	2.12E-02	1.33E-02	7.98E-03	4.55E-03	2.48E-03	1.30E-03	6.56E-04	3.21E-04	1.52E-04
	1.52E-01	1.42E-01	1.29E-01	1.13E-01	9.62E-02	7.82E-02	6.09E-02	4.51E-02	3.18E-02	2.13E-02	1.36E-02	8.25E-03	4.79E-03	2.67E-03	1.43E-03	7.45E-04	3.77E-04
	1.30E-01	1.29E-01	1.25E-01	1.17E-01	1.06E-01	9.15E-02	7.58E-02	5.98E-02	4.49E-02	3.20E-02	2.17E-02	1.40E-02	8.67E-03	5.14E-03	2.94E-03	1.63E-03	8.76E-04
	1.05E-01	1.11E-01	1.14E-01	1.13E-01	1.09E-01	1.00E-01	8.86E-02	7.44E-02	5.94E-02	4.51E-02	3.26E-02	2.24E-02	1.47E-02	9.31E-03	5.67E-03	3.34E-03	1.91E-03
	7.89E-02	8.89E-02	9.74E-02	1.03E-01	1.06E-01	1.04E-01	9.73E-02	8.70E-02	7.40E-02	5.98E-02	4.59E-02	3.37E-02	2.36E-02	1.58E-02	1.03E-02	6.44E-03	3.93E-03
	5.59E-02	6.71E-02	7.83E-02	8.84E-02	9.62E-02	1.00E-01	1.00E-01	9.55E-02	8.65E-02	7.44E-02	6.09E-02	4.75E-02	3.54E-02	2.53E-02	1.75E-02	1.17E-02	7.57E-03
	3.73E-02	4.76E-02	5.91E-02	7.10E-02	8.23E-02	9.15E-02	9.73E-02	9.86E-02	9.50E-02	8.70E-02	7.58E-02	6.29E-02	4.99E-02	3.80E-02	2.79E-02	1.98E-02	1.37E-02
	2.33E-02	3.17E-02	4.19E-02	5.36E-02	6.61E-02	7.82E-02	8.86E-02	9.55E-02	9.80E-02	9.55E-02	8.86E-02	7.82E-02	6.61E-02	5.36E-02	4.19E-02	3.17E-02	2.33E-02
	1.37E-02	1.98E-02	2.79E-02	3.80E-02	4.99E-02	6.29E-02	7.58E-02	8.70E-02	9.50E-02	9.86E-02	9.73E-02	9.15E-02	8.23E-02	7.10E-02	5.91E-02	4.76E-02	3.73E-02
	7.57E-03	1.17E-02	1.75E-02	2.53E-02	3.54E-02	4.75E-02	6.09E-02	7.44E-02	8.65E-02	9.55E-02	1.00E-01	1.00E-01	9.62E-02	8.84E-02	7.83E-02	6.71E-02	5.59E-02
	3.93E-03	6.44E-03	1.03E-02	1.58E-02	2.36E-02	3.37E-02	4.59E-02	5.98E-02	7.40E-02	8.70E-02	9.73E-02	1.04E-01	1.06E-01	1.03E-01	9.74E-02	8.89E-02	7.89E-02
	1.91E-03	3.34E-03	5.67E-03	9.31E-03	1.47E-02	2.24E-02	3.26E-02	4.51E-02	5.94E-02	7.44E-02	8.86E-02	1.00E-01	1.09E-01	1.13E-01	1.14E-01	1.11E-01	1.05E-01
	8.76E-04	1.63E-03	2.94E-03	5.14E-03	8.67E-03	1.40E-02	2.17E-02	3.20E-02	4.49E-02	5.98E-02	7.58E-02	9.15E-02	1.06E-01	1.17E-01	1.25E-01	1.29E-01	1.30E-01
	3.77E-04	7.45E-04	1.43E-03	2.67E-03	4.79E-03	8.25E-03	1.36E-02	2.13E-02	3.18E-02	4.51E-02	6.09E-02	7.82E-02	9.62E-02	1.13E-01	1.29E-01	1.42E-01	1.52E-01
	1.52E-04	3.21E-04	6.56E-04	1.30E-03	2.48E-03	4.55E-03	7.98E-03	1.33E-02	2.12E-02	3.20E-02	4.59E-02	6.29E-02	8.23E-02	1.03E-01	1.25E-01	1.47E-01	1.67E-01
	5.78E-05	1.30E-04	2.82E-04	5.95E-04	1.21E-03	2.36E-03	4.41E-03	7.84E-03	1.33E-02	2.13E-02	3.26E-02	4.75E-02	6.61E-02	8.84E-02	1.14E-01	1.42E-01	1.72E-01
5	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	1.41E-01	1.20E-01	1.01E-01	8.39E-02	6.79E-02	5.38E-02	4.16E-02	3.14E-02	2.31E-02	1.66E-02	1.16E-02	7.89E-03	5.25E-03	3.42E-03	2.18E-03	1.36E-03	8.40E-04
	1.38E-01	1.23E-01	1.08E-01	9.27E-02	7.81E-02	6.44E-02	5.19E-02	4.08E-02	3.12E-02	2.33E-02	1.69E-02	1.20E-02	8.32E-03	5.64E-03	3.74E-03	2.44E-03	1.56E-03
	1.30E-01	1.20E-01	1.10E-01	9.84E-02	8.64E-02	7.41E-02	6.21E-02	5.08E-02	4.05E-02	3.14E-02	2.38E-02	1.76E-02	1.27E-02	8.93E-03	6.17E-03	4.18E-03	2.79E-03
	1.17E-01	1.13E-01	1.08E-01	1.00E-01	9.17E-02	8.19E-02	7.15E-02	6.08E-02	5.04E-02	4.08E-02	3.21E-02	2.47E-02	1.85E-02	1.36E-02	9.77E-03	6.89E-03	4.78E-03
	1.02E-01	1.03E-01	1.01E-01	9.84E-02	9.36E-02	8.70E-02	7.90E-02	7.00E-02	6.04E-02	5.08E-02	4.16E-02	3.33E-02	2.60E-02	1.99E-02	1.49E-02	1.09E-02	7.89E-03
	8.52E-02	8.92E-02	9.18E-02	9.27E-02	9.17E-02	8.87E-02	8.39E-02	7.73E-02	6.95E-02	6.08E-02	5.19E-02	4.32E-02	3.51E-02	2.79E-02	2.17E-02	1.66E-02	1.25E-02
	6.84E-02	7.45E-02	7.98E-02	8.39E-02	8.64E-02	8.70E-02	8.56E-02	8.21E-02	7.68E-02	7.00E-02	6.21E-02	5.38E-02	4.55E-02	3.77E-02	3.05E-02	2.43E-02	1.90E-02
	5.27E-02	5.98E-02	6.66E-02	7.29E-02	7.81E-02	8.19E-02	8.39E-02	8.38E-02	8.15E-02	7.73E-02	7.15E-02	6.44E-02	5.67E-02	4.89E-02	4.12E-02	3.41E-02	2.78E-02
	3.91E-02	4.61E-02	5.35E-02	6.09E-02	6.79E-02	7.41E-02	7.90E-02	8.21E-02	8.32E-02	8.21E-02	7.90E-02	7.41E-02	6.79E-02	6.09E-02	5.35E-02	4.61E-02	3.91E-02
	2.78E-02	3.41E-02	4.12E-02	4.89E-02	5.67E-02	6.44E-02	7.15E-02	7.73E-02	8.15E-02	8.38E-02	8.39E-02	8.19E-02	7.81E-02	7.29E-02	6.66E-02	5.98E-02	5.27E-02
	1.90E-02	2.43E-02	3.05E-02	3.77E-02	4.55E-02	5.38E-02	6.21E-02	7.00E-02	7.68E-02	8.21E-02	8.56E-02	8.70E-02	8.64E-02	8.39E-02	7.98E-02	7.45E-02	6.84E-02
	1.25E-02	1.66E-02	2.17E-02	2.79E-02	3.51E-02	4.32E-02	5.19E-02	6.08E-02	6.95E-02	7.73E-02	8.39E-02	8.87E-02	9.17E-02	9.27E-02	9.18E-02	8.92E-02	8.52E-02
	7.89E-03	1.09E-02	1.49E-02	1.99E-02	2.60E-02	3.33E-02	4.16E-02	5.08E-02	6.04E-02	7.00E-02	7.90E-02	8.70E-02	9.36E-02	9.84E-02	1.01E-01	1.03E-01	1.02E-01
	4.78E-03	6.89E-03	9.77E-03	1.36E-02	1.85E-02	2.47E-02	3.21E-02	4.08E-02	5.04E-02	6.08E-02	7.15E-02	8.19E-02	9.17E-02	1.00E-01	1.08E-01	1.13E-01	1.17E-01
	2.79E-03	4.18E-03	6.17E-03	8.93E-03	1.27E-02	1.76E-02	2.38E-02	3.14E-02	4.05E-02	5.08E-02	6.21E-02	7.41E-02	8.64E-02	9.84E-02	1.10E-01	1.20E-01	1.30E-01
	1.56E-03	2.44E-03	3.74E-03	5.64E-03	8.32E-03	1.20E-02	1.69E-02	2.33E-02	3.12E-02	4.08E-02	5.19E-02	6.44E-02	7.81E-02	9.27E-02	1.08E-01	1.23E-01	1.38E-01
	8.40E-04	1.36E-03	2.18E-03	3.42E-03	5.25E-03	7.89E-03	1.16E-02	1.66E-02	2.31E-02	3.14E-02	4.16E-02	5.38E-02	6.79E-02	8.39E-02	1.01E-01	1.20E-01	1.41E-01

Table 2-S. *Input modal composition mass fractions (by columns) in the nucleation mode and composition standard deviation for involatile core of 5%.*

σ	modal composition																
1	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	5.13E-01	2.31E-01	4.88E-02	3.99E-03	1.20E-04	1.34E-06	5.47E-09	8.22E-12	4.55E-15	9.25E-19	6.93E-23	1.91E-27	1.93E-32	7.20E-38	9.91E-44	5.29E-50	1.32E-56
	3.11E-01	3.81E-01	2.19E-01	4.86E-02	3.99E-03	1.20E-04	1.34E-06	5.47E-09	8.22E-12	4.55E-15	9.25E-19	6.93E-23	1.91E-27	1.93E-32	7.23E-38	1.05E-43	7.12E-50
	6.95E-02	2.31E-01	3.61E-01	2.18E-01	4.86E-02	3.99E-03	1.20E-04	1.34E-06	5.47E-09	8.22E-12	4.55E-15	9.25E-19	6.93E-23	1.91E-27	1.94E-32	7.65E-38	1.41E-43
	5.70E-03	5.16E-02	2.19E-01	3.59E-01	2.18E-01	4.86E-02	3.99E-03	1.20E-04	1.34E-06	5.47E-09	8.22E-12	4.55E-15	9.25E-19	6.93E-23	1.92E-27	2.05E-32	1.03E-37
	1.72E-04	4.24E-03	4.88E-02	2.18E-01	3.59E-01	2.18E-01	4.86E-02	3.99E-03	1.20E-04	1.34E-06	5.47E-09	8.22E-12	4.55E-15	9.25E-19	6.96E-23	2.03E-27	2.76E-32
	1.91E-06	1.28E-04	4.01E-03	4.86E-02	2.18E-01	3.59E-01	2.18E-01	4.86E-02	3.99E-03	1.20E-04	1.34E-06	5.47E-09	8.22E-12	4.55E-15	9.29E-19	7.36E-23	2.73E-27
	7.82E-09	1.42E-06	1.21E-04	3.99E-03	4.86E-02	2.18E-01	3.59E-01	2.18E-01	4.86E-02	3.99E-03	1.20E-04	1.34E-06	5.47E-09	8.22E-12	4.57E-15	9.83E-19	9.90E-23
	1.18E-11	5.81E-09	1.34E-06	1.20E-04	3.99E-03	4.86E-02	2.18E-01	3.59E-01	2.18E-01	4.86E-02	3.99E-03	1.20E-04	1.34E-06	5.47E-09	8.26E-12	4.83E-15	1.32E-18
	6.50E-15	8.73E-12	5.49E-09	1.34E-06	1.20E-04	3.99E-03	4.86E-02	2.18E-01	3.59E-01	2.18E-01	4.86E-02	3.99E-03	1.20E-04	1.34E-06	5.49E-09	8.73E-12	6.50E-15
	1.32E-18	4.83E-15	8.26E-12	5.47E-09	1.34E-06	1.20E-04	3.99E-03	4.86E-02	2.18E-01	3.59E-01	2.18E-01	4.86E-02	3.99E-03	1.20E-04	1.34E-06	5.81E-09	1.18E-11
	9.90E-23	9.83E-19	4.57E-15	8.22E-12	5.47E-09	1.34E-06	1.20E-04	3.99E-03	4.86E-02	2.18E-01	3.59E-01	2.18E-01	4.86E-02	3.99E-03	1.21E-04	1.42E-06	7.82E-09
	2.73E-27	7.36E-23	9.29E-19	4.55E-15	8.22E-12	5.47E-09	1.34E-06	1.20E-04	3.99E-03	4.86E-02	2.18E-01	3.59E-01	2.18E-01	4.86E-02	4.01E-03	1.28E-04	1.91E-06
	2.76E-32	2.03E-27	6.96E-23	9.25E-19	4.55E-15	8.22E-12	5.47E-09	1.34E-06	1.20E-04	3.99E-03	4.86E-02	2.18E-01	3.59E-01	2.18E-01	4.88E-02	4.24E-03	1.72E-04
	1.03E-37	2.05E-32	1.92E-27	6.93E-23	9.25E-19	4.55E-15	8.22E-12	5.47E-09	1.34E-06	1.20E-04	3.99E-03	4.86E-02	2.18E-01	3.59E-01	2.19E-01	5.16E-02	5.70E-03
	1.41E-43	7.65E-38	1.94E-32	1.91E-27	6.93E-23	9.25E-19	4.55E-15	8.22E-12	5.47E-09	1.34E-06	1.20E-04	3.99E-03	4.86E-02	2.18E-01	3.61E-01	2.31E-01	6.95E-02
	7.12E-50	1.05E-43	7.23E-38	1.93E-32	1.91E-27	6.93E-23	9.25E-19	4.55E-15	8.22E-12	5.47E-09	1.34E-06	1.20E-04	3.99E-03	4.86E-02	2.19E-01	3.81E-01	3.11E-01
	1.32E-56	5.29E-50	9.91E-44	7.20E-38	1.93E-32	1.91E-27	6.93E-23	9.25E-19	4.55E-15	8.22E-12	5.47E-09	1.34E-06	1.20E-04	3.99E-03	4.88E-02	2.31E-01	5.13E-01
	9.00E-001																
2	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	2.99E-01	2.04E-01	1.21E-01	6.06E-02	2.46E-02	7.91E-03	2.00E-03	3.93E-04	6.02E-05	7.19E-06	6.69E-07	4.86E-08	2.77E-09	1.25E-10	4.58E-12	1.41E-13	3.79E-15
	2.64E-01	2.31E-01	1.77E-01	1.13E-01	5.90E-02	2.44E-02	7.89E-03	1.99E-03	3.93E-04	6.02E-05	7.20E-06	6.71E-07	4.90E-08	2.84E-09	1.34E-10	5.30E-12	1.83E-13
	1.82E-01	2.04E-01	2.00E-01	1.65E-01	1.10E-01	5.84E-02	2.43E-02	7.89E-03	1.99E-03	3.93E-04	6.03E-05	7.21E-06	6.77E-07	5.04E-08	3.05E-09	1.55E-10	6.85E-12
	9.72E-02	1.40E-01	1.77E-01	1.87E-01	1.60E-01	1.09E-01	5.83E-02	2.43E-02	7.89E-03	1.99E-03	3.93E-04	6.04E-05	7.28E-06	6.96E-07	5.40E-08	3.52E-09	2.00E-10
	4.05E-02	7.51E-02	1.21E-01	1.65E-01	1.82E-01	1.59E-01	1.09E-01	5.83E-02	2.43E-02	7.89E-03	2.00E-03	3.94E-04	6.09E-05	7.48E-06	7.46E-07	6.25E-08	4.56E-09
	1.32E-02	3.13E-02	6.50E-02	1.13E-01	1.60E-01	1.80E-01	1.59E-01	1.09E-01	5.83E-02	2.43E-02	7.89E-03	2.00E-03	3.97E-04	6.26E-05	8.02E-06	8.62E-07	8.08E-08
	3.33E-03	1.02E-02	2.71E-02	6.06E-02	1.10E-01	1.59E-01	1.80E-01	1.58E-01	1.09E-01	5.83E-02	2.43E-02	7.91E-03	2.02E-03	4.08E-04	6.72E-05	9.27E-06	1.12E-06
	6.55E-04	2.57E-03	8.80E-03	2.53E-02	5.90E-02	1.09E-01	1.59E-01	1.80E-01	1.58E-01	1.09E-01	5.83E-02	2.44E-02	7.98E-03	2.07E-03	4.38E-04	7.76E-05	1.20E-05
	1.00E-04	5.06E-04	2.22E-03	8.20E-03	2.46E-02	5.84E-02	1.09E-01	1.58E-01	1.80E-01	1.58E-01	1.09E-01	5.84E-02	2.46E-02	8.20E-03	2.22E-03	5.06E-04	1.00E-04
	1.20E-05	7.76E-05	4.38E-04	2.07E-03	7.98E-03	2.44E-02	5.83E-02	1.09E-01	1.58E-01	1.80E-01	1.59E-01	1.09E-01	5.90E-02	2.53E-02	8.80E-03	2.57E-03	6.55E-04
	1.12E-06	9.27E-06	6.72E-05	4.08E-04	2.02E-03	7.91E-03	2.43E-02	5.83E-02	1.09E-01	1.58E-01	1.80E-01	1.59E-01	1.10E-01	6.06E-02	2.71E-02	1.02E-02	3.33E-03
	8.08E-08	8.62E-07	8.02E-06	6.26E-05	3.97E-04	2.00E-03	7.89E-03	2.43E-02	5.83E-02	1.09E-01	1.59E-01	1.80E-01	1.60E-01	1.13E-01	6.50E-02	3.13E-02	1.32E-02
	4.56E-09	6.25E-08	7.46E-07	7.48E-06	6.09E-05	3.94E-04	2.00E-03	7.89E-03	2.43E-02	5.83E-02	1.09E-01	1.59E-01	1.82E-01	1.65E-01	1.21E-01	7.51E-02	4.05E-02
	2.00E-10	3.52E-09	5.40E-08	6.96E-07	7.28E-06	6.04E-05	3.93E-04	1.99E-03	7.89E-03	2.43E-02	5.83E-02	1.09E-01	1.60E-01	1.87E-01	1.77E-01	1.40E-01	9.72E-02
	6.85E-12	1.55E-10	3.05E-09	5.04E-08	6.77E-07	7.21E-06	6.03E-05	3.93E-04	1.99E-03	7.89E-03	2.43E-02	5.84E-02	1.10E-01	1.65E-01	2.00E-01	2.04E-01	1.82E-01
	1.83E-13	5.30E-12	1.34E-10	2.84E-09	4.90E-08	6.71E-07	7.20E-06	6.02E-05	3.93E-04	1.99E-03	7.89E-03	2.44E-02	5.90E-02	1.13E-01	1.77E-01	2.31E-01	2.64E-01
	3.79E-15	1.41E-13	4.58E-12	1.25E-10	2.77E-09	4.86E-08	6.69E-07	7.19E-06	6.02E-05	3.93E-04	2.00E-03	7.91E-03	2.46E-02	6.06E-02	1.21E-01	2.04E-01	2.99E-01
3	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	2.11E-01	1.64E-01	1.20E-01	8.25E-02	5.27E-02	3.09E-02	1.64E-02	7.92E-03	3.43E-03	1.34E-03	4.70E-04	1.49E-04	4.30E-05	1.14E-05	2.80E-06	6.44E-07	1.41E-07
	2.00E-01	1.73E-01	1.42E-01	1.09E-01	7.77E-02	5.09E-02	3.03E-02	1.63E-02	7.90E-03	3.44E-03	1.35E-03	4.78E-04	1.54E-04	4.57E-05	1.25E-05	3.23E-06	7.87E-07
	1.69E-01	1.64E-01	1.50E-01	1.29E-01	1.03E-01	7.51E-02	5.00E-02	3.00E-02	1.63E-02	7.92E-03	3.47E-03	1.37E-03	4.95E-04	1.64E-04	5.03E-05	1.45E-05	3.94E-06
	1.28E-01	1.38E-01	1.42E-01	1.36E-01	1.21E-01	9.91E-02	7.37E-02	4.95E-02	3.00E-02	1.63E-02	7.99E-03	3.53E-03	1.42E-03	5.26E-04	1.80E-04	5.80E-05	1.77E-05
	8.69E-02	1.05E-01	1.20E-01	1.29E-01	1.28E-01	1.17E-01	9.73E-02	7.31E-02	4.94E-02	3.00E-02	1.64E-02	8.13E-03	3.66E-03	1.51E-03	5.79E-04	2.08E-04	7.09E-05
	5.27E-02	7.11E-02	9.09E-02	1.09E-01	1.21E-01	1.24E-01	1.15E-01	9.65E-02	7.29E-02	4.95E-02	3.03E-02	1.67E-02	8.42E-03	3.89E-03	1.66E-03	6.68E-04	2.54E-04
	2.86E-02	4.31E-02	6.16E-02	8.25E-02	1.03E-01	1.17E-01	1.22E-01	1.14E-01	9.63E-02	7.31E-02	5.00E-02	3.09E-02	1.73E-02	8.95E-03	4.28E-03	1.92E-03	8.17E-04
	1.39E-02	2.34E-02	3.74E-02	5.59E-02	7.77E-02	9.91E-02	1.15E-01	1.20E-01	1.14E-01	9.65E-02	7.37E-02	5.09E-02	3.19E-02	1.84E-02	9.85E-03	4.94E-03	2.35E-03
	6.04E-03	1.14E-02	2.03E-02	3.39E-02	5.27E-02	7.51E-02	9.73E-02	1.14E-01	1.20E-01	1.14E-01	9.73E-02	7.51E-02	5.27E-02	3.39E-02	2.03E-02	1.14E-02	6.04E-03
	2.35E-03	4.94E-03	9.85E-03	1.84E-02	3.19E-02	5.09E-02	7.37E-02	9.65E-02	1.14E-01	1.20E-01	1.15E-01	9.91E-02	7.77E-02	5.59E-02	3.74E-02	2.34E-02	1.39E-02
	8.17E-04	1.92E-03	4.28E-03	8.95E-03	1.73E-02	3.09E-02	5.00E-02	7.31E-02	9.63E-02	1.14E-01	1.22E-01	1.17E-01	1.03E-01	8.25E-02	6.16E-02	4.31E-02	2.86E-02
	2.54E-04	6.68E-04	1.66E-03	3.89E-03	8.42E-03	1.67E-02	3.03E-02	4.95E-02	7.29E-02	9.65E-02	1.15E-01	1.24E-01	1.21E-01	1.09E-01	9.09E-02	7.11E-02	5.27E-02
	7.09E-05	2.08E-04	5.79E-04	1.51E-03	3.66E-03	8.13E-03	1.64E-02	3.00E-02	4.94E-02	7.31E-02	9.73E-02	1.17E-01	1.28E-01	1.29E-01	1.20E-01	1.05E-01	8.69E-02
	1.77E-05	5.80E-05	1.80E-04	5.26E-04	1.42E-03	3.53E-03	7.99E-03	1.63E-02	3.00E-02	4.95E-02	7.37E-02	9.91E-02	1.21E-01	1.36E-01	1.42E-01	1.38E-01	1.28E-01
	3.94E-06	1.45E-05	5.03E-05	1.64E-04	4.95E-04	1.37E-03	3.47E-03	7.92E-03	1.63E-02	3.00E-02	5.00E-02	7.51E-02	1.03E-01	1.29E-01	1.50E-01	1.64E-01	1.69E-01
	7.87E-07	3.23E-06	1.25E-05	4.57E-05	1.54E-04	4.78E-04	1.35E-03	3.44E-03	7.90E-03	1.63E-02	3.03E-02	5.09E-02	7.77E-02	1.09E-01	1.42E-01	1.73E-01	2.00E-01
	1.41E-07	6.44E-07	2.80E-06	1.14E-05	4.30E-05	1.49E-04	4.70E-04	1.34E-03	3.43E-03	7.92E-03	1.64E-02	3.09E-02	5.27E-02	8.25E-02	1.20E-01	1.64E-01	2.11E-01
4	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	1.63E-01	1.35E-01	1.08E-01	8.37E-02	6.26E-02	4.50E-02	3.09E-02	2.02E-02	1.26E-02	7.43E-03	4.18E-03	2.24E-03	1.15E-03	5.64E-04	2.67E-04	1.23E-04	5.48E-05
	1.58E-01	1.39E-01	1.18E-01	9.79E-02	7.79E-02	5.96E-02	4.35E-02	3.03E-02	2.01E-02	1.26E-02	7.56E-03	4.31E-03	2.35E-03	1.23E-03	6.22E-04	3.04E-04	1.44E-04
	1.44E-01	1.35E-01	1.22E-01	1.07E-01	9.11E-02	7.41E-02	5.77E-02	4.27E-02	3.01E-02	2.02E-02	1.29E-02	7.81E-03	4.54E-03	2.53E-03	1.36E-03	7.06E-04	3.57E-04
	1.23E-01	1.23E-01	1.18E-01	1.11E-01	1.00E-01	8.67E-02	7.18E-02	5.66E-02	4.25E-02	3.03E-02	2.06E-02	1.33E-02	8.21E-03	4.87E-03	2.79E-03	1.54E-03	8.30E-04
	9.90E-02	1.05E-01	1.08E-01	1.07E-01	1.03E-01	9.52E-02	8.39E-02	7.05E-02	5.63E-02	4.27E-02	3.09E-02	2.12E-02	1.40E-02	8.82E-03	5.37E-03	3.16E-03	1.81E-03
	7.47E-02	8.42E-02	9.23E-02	9.79E-02	1.00E-01	9.82E-02	9.21E-02	8.24E-02	7.01E-02	5.66E-02	4.35E-02	3.19E-02	2.23E-02	1.50E-02	9.72E-03	6.10E-03	3.72E-03
	5.30E-02	6.36E-02	7.41E-02	8.37E-02	9.11E-02	9.52E-02	9.51E-02	9.05E-02	8.19E-02	7.05E-02	5.77E-02	4.50E-02	3.35E-02	2.40E-02	1.65E-02	1.10E-02	7.17E-03
	3.53E-02	4.51E-02	5.60E-02	6.73E-02	7.79E-02	8.67E-02	9.21E-02	9.34E-02	9.00E-02	8.24E-02	7.18E-02	5.96E-02	4.73E-02	3.60E-02	2.64E-02	1.88E-02	1.30E-02
	2.21E-02	3.00E-02	3.97E-02	5.08E-02	6.26E-02	7.41E-02	8.39E-02	9.05E-02	9.28E-02	9.05E-02	8.39E-02	7.41E-02	6.26E-02	5.08E-02	3.97E-02	3.00E-02	2.21E-02
	1.30E-02	1.88E-02	2.64E-02	3.60E-02	4.73E-02	5.96E-02	7.18E-02	8.24E-02	9.00E-02	9.34E-02	9.21E-02	8.67E-02	7.79E-02	6.73E-02	5.60E-02	4.51E-02	3.53E-02
	7.17E-03	1.10E-02	1.65E-02	2.40E-02	3.35E-02	4.50E-02	5.77E-02	7.05E-02	8.19E-02	9.05E-02	9.51E-02	9.52E-02	9.11E-02	8.37E-02	7.41E-02	6.36E-02	5.30E-02
	3.72E-03	6.10E-03	9.72E-03	1.50E-02	2.23E-02	3.19E-02	4.35E-02	5.66E-02	7.01E-02	8.24E-02	9.21E-02	9.82E-02	1.00E-01	9.79E-02	9.23E-02	8.42E-02	7.47E-02
	1.81E-03	3.16E-03	5.37E-03	8.82E-03	1.40E-02	2.12E-02	3.09E-02	4.27E-02	5.63E-02	7.05E-02	8.39E-02	9.52E-02	1.03E-01	1.07E-01	1.08E-01	1.05E-01	9.90E-02
	8.30E-04	1.54E-03	2.79E-03	4.87E-03	8.21E-03	1.33E-02	2.06E-02	3.03E-02	4.25E-02	5.66E-02	7.18E-02	8.67E-02	1.00E-01	1.11E-01	1.18E-01	1.23E-01	1.23E-01
	3.57E-04	7.06E-04	1.36E-03	2.53E-03	4.54E-03	7.81E-03	1.29E-02	2.02E-02	3.01E-02	4.27E-02	5.77E-02	7.41E-02	9.11E-02	1.07E-01	1.22E-01	1.35E-01	1.44E-01
	1.44E-04	3.04E-04	6.22E-04	1.23E-03	2.35E-03	4.31E-03	7.56E-03	1.26E-02	2.01E-02	3.03E-02	4.35E-02	5.96E-02	7.79E-02	9.79E-02	1.18E-01	1.39E-01	1.58E-01
	5.48E-05	1.23E-04	2.67E-04	5.64E-04	1.15E-03	2.24E-03	4.18E-03	7.43E-03	1.26E-02	2.02E-02	3.09E-02	4.50E-02	6.26E-02	8.37E-02	1.08E-01	1.35E-01	1.63E-01
5	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	1.33E-01	1.14E-01	9.61E-02	7.94E-02	6.44E-02	5.10E-02	3.95E-02	2.98E-02	2.19E-02	1.57E-02	1.10E-02	7.48E-03	4.98E-03	3.24E-03	2.07E-03	1.29E-03	7.96E-04
	1.30E-01	1.16E-01	1.02E-01	8.78E-02	7.40E-02	6.11E-02	4.92E-02	3.86E-02	2.96E-02	2.21E-02	1.60E-02	1.14E-02	7.88E-03	5.34E-03	3.54E-03	2.31E-03	1.48E-03
	1.23E-01	1.14E-01	1.04E-01	9.32E-02	8.18E-02	7.02E-02	5.89E-02	4.81E-02	3.84E-02	2.98E-02	2.25E-02	1.66E-02	1.20E-02	8.46E-03	5.84E-03	3.96E-03	2.64E-03
	1.11E-01	1.07E-01	1.02E-01	9.51E-02	8.69E-02	7.76E-02	6.77E-02	5.76E-02	4.78E-02	3.86E-02	3.04E-02	2.34E-02	1.75E-02	1.29E-02	9.26E-03	6.53E-03	4.53E-03
	9.67E-02	9.72E-02	9.61E-02	9.32E-02	8.86E-02	8.24E-02	7.48E-02	6.63E-02	5.72E-02	4.81E-02	3.95E-02	3.16E-02	2.46E-02	1.88E-02	1.41E-02	1.03E-02	7.47E-03
	8.07E-02	8.45E-02	8.69E-02	8.78E-02	8.69E-02	8.41E-02	7.95E-02	7.32E-02	6.58E-02	5.76E-02	4.92E-02	4.09E-02	3.33E-02	2.64E-02	2.06E-02	1.57E-02	1.18E-02
	6.48E-02	7.06E-02	7.56E-02	7.94E-02	8.18E-02	8.24E-02	8.11E-02	7.78E-02	7.27E-02	6.63E-02	5.89E-02	5.10E-02	4.31E-02	3.57E-02	2.89E-02	2.30E-02	1.80E-02
	5.00E-02	5.66E-02	6.31E-02	6.91E-02	7.40E-02	7.76E-02	7.95E-02	7.93E-02	7.72E-02	7.32E-02	6.77E-02	6.11E-02	5.38E-02	4.63E-02	3.91E-02	3.24E-02	2.63E-02
	3.70E-02	4.37E-02	5.07E-02	5.77E-02	6.44E-02	7.02E-02	7.48E-02	7.78E-02	7.88E-02	7.78E-02	7.48E-02	7.02E-02	6.44E-02	5.77E-02	5.07E-02	4.37E-02	3.70E-02
	2.63E-02	3.24E-02	3.91E-02	4.63E-02	5.38E-02	6.11E-02	6.77E-02	7.32E-02	7.72E-02	7.93E-02	7.95E-02	7.76E-02	7.40E-02	6.91E-02	6.31E-02	5.66E-02	5.00E-02
	1.80E-02	2.30E-02	2.89E-02	3.57E-02	4.31E-02	5.10E-02	5.89E-02	6.63E-02	7.27E-02	7.78E-02	8.11E-02	8.24E-02	8.18E-02	7.94E-02	7.56E-02	7.06E-02	6.48E-02
	1.18E-02	1.57E-02	2.06E-02	2.64E-02	3.33E-02	4.09E-02	4.92E-02	5.76E-02	6.58E-02	7.32E-02	7.95E-02	8.41E-02	8.69E-02	8.78E-02	8.69E-02	8.45E-02	8.07E-02
	7.47E-03	1.03E-02	1.41E-02	1.88E-02	2.46E-02	3.16E-02	3.95E-02	4.81E-02	5.72E-02	6.63E-02	7.48E-02	8.24E-02	8.86E-02	9.32E-02	9.61E-02	9.72E-02	9.67E-02
	4.53E-03	6.53E-03	9.26E-03	1.29E-02	1.75E-02	2.34E-02	3.04E-02	3.86E-02	4.78E-02	5.76E-02	6.77E-02	7.76E-02	8.69E-02	9.51E-02	1.02E-01	1.07E-01	1.11E-01
	2.64E-03	3.96E-03	5.84E-03	8.46E-03	1.20E-02	1.66E-02	2.25E-02	2.98E-02	3.84E-02	4.81E-02	5.89E-02	7.02E-02	8.18E-02	9.32E-02	1.04E-01	1.14E-01	1.23E-01
	1.48E-03	2.31E-03	3.54E-03	5.34E-03	7.88E-03	1.14E-02	1.60E-02	2.21E-02	2.96E-02	3.86E-02	4.92E-02	6.11E-02	7.40E-02	8.78E-02	1.02E-01	1.16E-01	1.30E-01
	7.96E-04	1.29E-03	2.07E-03	3.24E-03	4.98E-03	7.48E-03	1.10E-02	1.57E-02	2.19E-02	2.98E-02	3.95E-02	5.10E-02	6.44E-02	7.94E-02	9.61E-02	1.14E-01	1.33E-01

Table 3-S. *Input modal composition mass fractions (by columns) in the nucleation mode and composition standard deviation for involatile core of 10%.*

σ	modal composition																
1	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	5.70E-02	2.57E-02	5.42E-03	4.43E-04	1.34E-05	1.49E-07	6.08E-10	9.13E-13	5.05E-16	1.03E-19	7.69E-24	2.12E-28	2.15E-33	8.00E-39	1.10E-44	5.87E-51	1.47E-57
	3.46E-02	4.24E-02	2.43E-02	5.40E-03	4.43E-04	1.34E-05	1.49E-07	6.08E-10	9.13E-13	5.05E-16	1.03E-19	7.69E-24	2.12E-28	2.15E-33	8.04E-39	1.16E-44	7.91E-51
	7.72E-03	2.57E-02	4.01E-02	2.42E-02	5.40E-03	4.43E-04	1.34E-05	1.49E-07	6.08E-10	9.13E-13	5.05E-16	1.03E-19	7.69E-24	2.12E-28	2.16E-33	8.50E-39	1.57E-44
	6.34E-04	5.73E-03	2.43E-02	3.99E-02	2.42E-02	5.40E-03	4.43E-04	1.34E-05	1.49E-07	6.08E-10	9.13E-13	5.05E-16	1.03E-19	7.70E-24	2.13E-28	2.28E-33	1.14E-38
	1.91E-05	4.71E-04	5.42E-03	2.42E-02	3.99E-02	2.42E-02	5.40E-03	4.43E-04	1.34E-05	1.49E-07	6.08E-10	9.13E-13	5.05E-16	1.03E-19	7.73E-24	2.25E-28	3.07E-33
	2.13E-07	1.42E-05	4.45E-04	5.40E-03	2.42E-02	3.99E-02	2.42E-02	5.40E-03	4.43E-04	1.34E-05	1.49E-07	6.08E-10	9.13E-13	5.05E-16	1.03E-19	8.17E-24	3.03E-28
	8.69E-10	1.58E-07	1.34E-05	4.43E-04	5.40E-03	2.42E-02	3.99E-02	2.42E-02	5.40E-03	4.43E-04	1.34E-05	1.49E-07	6.08E-10	9.14E-13	5.08E-16	1.09E-19	1.10E-23
	1.31E-12	6.45E-10	1.49E-07	1.34E-05	4.43E-04	5.40E-03	2.42E-02	3.99E-02	2.42E-02	5.40E-03	4.43E-04	1.34E-05	1.49E-07	6.08E-10	9.18E-13	5.37E-16	1.47E-19
	7.22E-16	9.70E-13	6.10E-10	1.49E-07	1.34E-05	4.43E-04	5.40E-03	2.42E-02	3.99E-02	2.42E-02	5.40E-03	4.43E-04	1.34E-05	1.49E-07	6.10E-10	9.70E-13	7.22E-16
	1.47E-19	5.37E-16	9.18E-13	6.08E-10	1.49E-07	1.34E-05	4.43E-04	5.40E-03	2.42E-02	3.99E-02	2.42E-02	5.40E-03	4.43E-04	1.34E-05	1.49E-07	6.45E-10	1.31E-12
	1.10E-23	1.09E-19	5.08E-16	9.14E-13	6.08E-10	1.49E-07	1.34E-05	4.43E-04	5.40E-03	2.42E-02	3.99E-02	2.42E-02	5.40E-03	4.43E-04	1.34E-05	1.58E-07	8.69E-10
	3.03E-28	8.17E-24	1.03E-19	5.05E-16	9.13E-13	6.08E-10	1.49E-07	1.34E-05	4.43E-04	5.40E-03	2.42E-02	3.99E-02	2.42E-02	5.40E-03	4.45E-04	1.42E-05	2.13E-07
	3.07E-33	2.25E-28	7.73E-24	1.03E-19	5.05E-16	9.13E-13	6.08E-10	1.49E-07	1.34E-05	4.43E-04	5.40E-03	2.42E-02	3.99E-02	2.42E-02	5.42E-03	4.71E-04	1.91E-05
	1.14E-38	2.28E-33	2.13E-28	7.70E-24	1.03E-19	5.05E-16	9.13E-13	6.08E-10	1.49E-07	1.34E-05	4.43E-04	5.40E-03	2.42E-02	3.99E-02	2.43E-02	5.73E-03	6.34E-04
	1.57E-44	8.50E-39	2.16E-33	2.12E-28	7.69E-24	1.03E-19	5.05E-16	9.13E-13	6.08E-10	1.49E-07	1.34E-05	4.43E-04	5.40E-03	2.42E-02	4.01E-02	2.57E-02	7.72E-03
	7.91E-51	1.16E-44	8.04E-39	2.15E-33	2.12E-28	7.69E-24	1.03E-19	5.05E-16	9.13E-13	6.08E-10	1.49E-07	1.34E-05	4.43E-04	5.40E-03	2.43E-02	4.24E-02	3.46E-02
	1.47E-57	5.87E-51	1.10E-44	8.00E-39	2.15E-33	2.12E-28	7.69E-24	1.03E-19	5.05E-16	9.13E-13	6.08E-10	1.49E-07	1.34E-05	4.43E-04	5.42E-03	2.57E-02	5.70E-02
2	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	3.33E-02	2.27E-02	1.35E-02	6.74E-03	2.73E-03	8.79E-04	2.22E-04	4.36E-05	6.69E-06	7.99E-07	7.44E-08	5.40E-09	3.07E-10	1.39E-11	5.09E-13	1.57E-14	4.21E-16
	2.94E-02	2.57E-02	1.96E-02	1.26E-02	6.55E-03	2.71E-03	8.77E-04	2.22E-04	4.36E-05	6.69E-06	8.00E-07	7.45E-08	5.45E-09	3.16E-10	1.49E-11	5.89E-13	2.03E-14
	2.02E-02	2.27E-02	2.22E-02	1.83E-02	1.22E-02	6.49E-03	2.70E-03	8.76E-04	2.22E-04	4.36E-05	6.69E-06	8.01E-07	7.52E-08	5.60E-09	3.39E-10	1.72E-11	7.62E-13
	1.08E-02	1.56E-02	1.96E-02	2.07E-02	1.78E-02	1.21E-02	6.48E-03	2.70E-03	8.76E-04	2.22E-04	4.37E-05	6.71E-06	8.08E-07	7.73E-08	6.00E-09	3.92E-10	2.23E-11
	4.50E-03	8.35E-03	1.35E-02	1.83E-02	2.02E-02	1.77E-02	1.21E-02	6.48E-03	2.70E-03	8.76E-04	2.22E-04	4.38E-05	6.77E-06	8.31E-07	8.29E-08	6.94E-09	5.07E-10
	1.46E-03	3.48E-03	7.22E-03	1.26E-02	1.78E-02	2.00E-02	1.76E-02	1.21E-02	6.48E-03	2.70E-03	8.77E-04	2.22E-04	4.41E-05	6.96E-06	8.91E-07	9.58E-08	8.98E-09
	3.69E-04	1.13E-03	3.01E-03	6.74E-03	1.22E-02	1.77E-02	2.00E-02	1.76E-02	1.21E-02	6.48E-03	2.70E-03	8.79E-04	2.24E-04	4.54E-05	7.46E-06	1.03E-06	1.24E-07
	7.28E-05	2.86E-04	9.77E-04	2.81E-03	6.55E-03	1.21E-02	1.76E-02	1.99E-02	1.76E-02	1.21E-02	6.48E-03	2.71E-03	8.87E-04	2.30E-04	4.87E-05	8.63E-06	1.33E-06
	1.12E-05	5.62E-05	2.47E-04	9.11E-04	2.73E-03	6.49E-03	1.21E-02	1.76E-02	1.99E-02	1.76E-02	1.21E-02	6.49E-03	2.73E-03	9.11E-04	2.47E-04	5.62E-05	1.12E-05
	1.33E-06	8.63E-06	4.87E-05	2.30E-04	8.87E-04	2.71E-03	6.48E-03	1.21E-02	1.76E-02	1.99E-02	1.76E-02	1.21E-02	6.55E-03	2.81E-03	9.77E-04	2.86E-04	7.28E-05
	1.24E-07	1.03E-06	7.46E-06	4.54E-05	2.24E-04	8.79E-04	2.70E-03	6.48E-03	1.21E-02	1.76E-02	2.00E-02	1.77E-02	1.22E-02	6.74E-03	3.01E-03	1.13E-03	3.69E-04
	8.98E-09	9.58E-08	8.91E-07	6.96E-06	4.41E-05	2.22E-04	8.77E-04	2.70E-03	6.48E-03	1.21E-02	1.76E-02	2.00E-02	1.78E-02	1.26E-02	7.22E-03	3.48E-03	1.46E-03
	5.07E-10	6.94E-09	8.29E-08	8.31E-07	6.77E-06	4.38E-05	2.22E-04	8.76E-04	2.70E-03	6.48E-03	1.21E-02	1.77E-02	2.02E-02	1.83E-02	1.35E-02	8.35E-03	4.50E-03
	2.23E-11	3.92E-10	6.00E-09	7.73E-08	8.08E-07	6.71E-06	4.37E-05	2.22E-04	8.76E-04	2.70E-03	6.48E-03	1.21E-02	1.78E-02	2.07E-02	1.96E-02	1.56E-02	1.08E-02
	7.62E-13	1.72E-11	3.39E-10	5.60E-09	7.52E-08	8.01E-07	6.69E-06	4.36E-05	2.22E-04	8.76E-04	2.70E-03	6.49E-03	1.22E-02	1.83E-02	2.22E-02	2.27E-02	2.02E-02
	2.03E-14	5.89E-13	1.49E-11	3.16E-10	5.45E-09	7.45E-08	8.00E-07	6.69E-06	4.36E-05	2.22E-04	8.77E-04	2.71E-03	6.55E-03	1.26E-02	1.96E-02	2.57E-02	2.94E-02
	4.21E-16	1.57E-14	5.09E-13	1.39E-11	3.07E-10	5.40E-09	7.44E-08	7.99E-07	6.69E-06	4.36E-05	2.22E-04	8.79E-04	2.73E-03	6.74E-03	1.35E-02	2.27E-02	3.33E-02
3	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	2.35E-02	1.82E-02	1.33E-02	9.17E-03	5.85E-03	3.43E-03	1.83E-03	8.80E-04	3.82E-04	1.49E-04	5.22E-05	1.66E-05	4.78E-06	1.26E-06	3.11E-07	7.16E-08	1.56E-08
	2.22E-02	1.92E-02	1.57E-02	1.21E-02	8.63E-03	5.65E-03	3.37E-03	1.81E-03	8.78E-04	3.82E-04	1.50E-04	5.32E-05	1.71E-05	5.07E-06	1.39E-06	3.59E-07	8.75E-08
	1.88E-02	1.82E-02	1.66E-02	1.43E-02	1.14E-02	8.34E-03	5.55E-03	3.34E-03	1.81E-03	8.80E-04	3.86E-04	1.53E-04	5.50E-05	1.82E-05	5.58E-06	1.61E-06	4.38E-07
	1.42E-02	1.54E-02	1.57E-02	1.51E-02	1.35E-02	1.10E-02	8.19E-03	5.50E-03	3.33E-03	1.81E-03	8.87E-04	3.93E-04	1.58E-04	5.85E-05	2.00E-05	6.44E-06	1.96E-06
	9.65E-03	1.17E-02	1.33E-02	1.43E-02	1.42E-02	1.30E-02	1.08E-02	8.12E-03	5.49E-03	3.34E-03	1.83E-03	9.04E-04	4.07E-04	1.68E-04	6.44E-05	2.31E-05	7.87E-06
	5.85E-03	7.90E-03	1.01E-02	1.21E-02	1.35E-02	1.37E-02	1.28E-02	1.07E-02	8.10E-03	5.50E-03	3.37E-03	1.86E-03	9.36E-04	4.32E-04	1.85E-04	7.43E-05	2.83E-05
	3.18E-03	4.79E-03	6.84E-03	9.17E-03	1.14E-02	1.30E-02	1.35E-02	1.27E-02	1.07E-02	8.12E-03	5.55E-03	3.43E-03	1.93E-03	9.94E-04	4.76E-04	2.13E-04	9.08E-05
	1.54E-03	2.60E-03	4.15E-03	6.22E-03	8.63E-03	1.10E-02	1.28E-02	1.34E-02	1.26E-02	1.07E-02	8.19E-03	5.65E-03	3.55E-03	2.05E-03	1.09E-03	5.49E-04	2.61E-04
	6.71E-04	1.26E-03	2.25E-03	3.77E-03	5.85E-03	8.34E-03	1.08E-02	1.27E-02	1.34E-02	1.27E-02	1.08E-02	8.34E-03	5.85E-03	3.77E-03	2.25E-03	1.26E-03	6.71E-04
	2.61E-04	5.49E-04	1.09E-03	2.05E-03	3.55E-03	5.65E-03	8.19E-03	1.07E-02	1.26E-02	1.34E-02	1.28E-02	1.10E-02	8.63E-03	6.22E-03	4.15E-03	2.60E-03	1.54E-03
	9.08E-05	2.13E-04	4.76E-04	9.94E-04	1.93E-03	3.43E-03	5.55E-03	8.12E-03	1.07E-02	1.27E-02	1.35E-02	1.30E-02	1.14E-02	9.17E-03	6.84E-03	4.79E-03	3.18E-03
	2.83E-05	7.43E-05	1.85E-04	4.32E-04	9.36E-04	1.86E-03	3.37E-03	5.50E-03	8.10E-03	1.07E-02	1.28E-02	1.37E-02	1.35E-02	1.21E-02	1.01E-02	7.90E-03	5.85E-03
	7.87E-06	2.31E-05	6.44E-05	1.68E-04	4.07E-04	9.04E-04	1.83E-03	3.34E-03	5.49E-03	8.12E-03	1.08E-02	1.30E-02	1.42E-02	1.43E-02	1.33E-02	1.17E-02	9.65E-03
	1.96E-06	6.44E-06	2.00E-05	5.85E-05	1.58E-04	3.93E-04	8.87E-04	1.81E-03	3.33E-03	5.50E-03	8.19E-03	1.10E-02	1.35E-02	1.51E-02	1.57E-02	1.54E-02	1.42E-02
	4.38E-07	1.61E-06	5.58E-06	1.82E-05	5.50E-05	1.53E-04	3.86E-04	8.80E-04	1.81E-03	3.34E-03	5.55E-03	8.34E-03	1.14E-02	1.43E-02	1.66E-02	1.82E-02	1.88E-02
	8.75E-08	3.59E-07	1.39E-06	5.07E-06	1.71E-05	5.32E-05	1.50E-04	3.82E-04	8.78E-04	1.81E-03	3.37E-03	5.65E-03	8.63E-03	1.21E-02	1.57E-02	1.92E-02	2.22E-02
	1.56E-08	7.16E-08	3.11E-07	1.26E-06	4.78E-06	1.66E-05	5.22E-05	1.49E-04	3.82E-04	8.80E-04	1.83E-03	3.43E-03	5.85E-03	9.17E-03	1.33E-02	1.82E-02	2.35E-02
4	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	1.81E-02	1.50E-02	1.20E-02	9.30E-03	6.96E-03	5.00E-03	3.43E-03	2.24E-03	1.40E-03	8.25E-04	4.64E-04	2.49E-04	1.27E-04	6.27E-05	2.97E-05	1.36E-05	6.08E-06
	1.76E-02	1.54E-02	1.32E-02	1.09E-02	8.66E-03	6.62E-03	4.84E-03	3.37E-03	2.23E-03	1.40E-03	8.40E-04	4.79E-04	2.61E-04	1.37E-04	6.91E-05	3.37E-05	1.60E-05
	1.60E-02	1.50E-02	1.36E-02	1.19E-02	1.01E-02	8.24E-03	6.41E-03	4.75E-03	3.35E-03	2.24E-03	1.43E-03	8.68E-04	5.04E-04	2.81E-04	1.51E-04	7.85E-05	3.97E-05
	1.37E-02	1.36E-02	1.32E-02	1.23E-02	1.11E-02	9.63E-03	7.97E-03	6.29E-03	4.72E-03	3.37E-03	2.28E-03	1.48E-03	9.13E-04	5.41E-04	3.10E-04	1.71E-04	9.23E-05
	1.10E-02	1.16E-02	1.20E-02	1.19E-02	1.15E-02	1.06E-02	9.32E-03	7.83E-03	6.26E-03	4.75E-03	3.43E-03	2.36E-03	1.55E-03	9.80E-04	5.97E-04	3.52E-04	2.02E-04
	8.30E-03	9.36E-03	1.03E-02	1.09E-02	1.11E-02	1.09E-02	1.02E-02	9.16E-03	7.79E-03	6.29E-03	4.84E-03	3.54E-03	2.48E-03	1.67E-03	1.08E-03	6.78E-04	4.13E-04
	5.89E-03	7.06E-03	8.24E-03	9.30E-03	1.01E-02	1.06E-02	1.06E-02	1.01E-02	9.10E-03	7.83E-03	6.41E-03	5.00E-03	3.72E-03	2.66E-03	1.84E-03	1.23E-03	7.97E-04
	3.92E-03	5.01E-03	6.22E-03	7.47E-03	8.66E-03	9.63E-03	1.02E-02	1.04E-02	1.00E-02	9.16E-03	7.97E-03	6.62E-03	5.25E-03	4.00E-03	2.94E-03	2.09E-03	1.44E-03
	2.45E-03	3.34E-03	4.41E-03	5.64E-03	6.96E-03	8.24E-03	9.32E-03	1.01E-02	1.03E-02	1.01E-02	9.32E-03	8.24E-03	6.96E-03	5.64E-03	4.41E-03	3.34E-03	2.45E-03
	1.44E-03	2.09E-03	2.94E-03	4.00E-03	5.25E-03	6.62E-03	7.97E-03	9.16E-03	1.00E-02	1.04E-02	1.02E-02	9.63E-03	8.66E-03	7.47E-03	6.22E-03	5.01E-03	3.92E-03
	7.97E-04	1.23E-03	1.84E-03	2.66E-03	3.72E-03	5.00E-03	6.41E-03	7.83E-03	9.10E-03	1.01E-02	1.06E-02	1.06E-02	1.01E-02	9.30E-03	8.24E-03	7.06E-03	5.89E-03
	4.13E-04	6.78E-04	1.08E-03	1.67E-03	2.48E-03	3.54E-03	4.84E-03	6.29E-03	7.79E-03	9.16E-03	1.02E-02	1.09E-02	1.11E-02	1.09E-02	1.03E-02	9.36E-03	8.30E-03
	2.02E-04	3.52E-04	5.97E-04	9.80E-04	1.55E-03	2.36E-03	3.43E-03	4.75E-03	6.26E-03	7.83E-03	9.32E-03	1.06E-02	1.15E-02	1.19E-02	1.20E-02	1.16E-02	1.10E-02
	9.23E-05	1.71E-04	3.10E-04	5.41E-04	9.13E-04	1.48E-03	2.28E-03	3.37E-03	4.72E-03	6.29E-03	7.97E-03	9.63E-03	1.11E-02	1.23E-02	1.32E-02	1.36E-02	1.37E-02
	3.97E-05	7.85E-05	1.51E-04	2.81E-04	5.04E-04	8.68E-04	1.43E-03	2.24E-03	3.35E-03	4.75E-03	6.41E-03	8.24E-03	1.01E-02	1.19E-02	1.36E-02	1.50E-02	1.60E-02
	1.60E-05	3.37E-05	6.91E-05	1.37E-04	2.61E-04	4.79E-04	8.40E-04	1.40E-03	2.23E-03	3.37E-03	4.84E-03	6.62E-03	8.66E-03	1.09E-02	1.32E-02	1.54E-02	1.76E-02
	6.08E-06	1.36E-05	2.97E-05	6.27E-05	1.27E-04	2.49E-04	4.64E-04	8.25E-04	1.40E-03	2.24E-03	3.43E-03	5.00E-03	6.96E-03	9.30E-03	1.20E-02	1.50E-02	1.81E-02
5	$C_{16}H_{34}$	$C_{17}H_{36}$	$C_{18}H_{38}$	$C_{19}H_{40}$	$C_{20}H_{42}$	$C_{21}H_{44}$	$C_{22}H_{46}$	$C_{23}H_{48}$	$C_{24}H_{50}$	$C_{25}H_{52}$	$C_{26}H_{54}$	$C_{27}H_{56}$	$C_{28}H_{58}$	$C_{29}H_{60}$	$C_{30}H_{62}$	$C_{31}H_{64}$	$C_{32}H_{66}$
	1.48E-02	1.27E-02	1.07E-02	8.83E-03	7.15E-03	5.67E-03	4.38E-03	3.31E-03	2.43E-03	1.74E-03	1.22E-03	8.31E-04	5.53E-04	3.60E-04	2.29E-04	1.44E-04	8.84E-05
	1.45E-02	1.29E-02	1.13E-02	9.76E-03	8.23E-03	6.78E-03	5.46E-03	4.29E-03	3.29E-03	2.45E-03	1.78E-03	1.26E-03	8.76E-04	5.93E-04	3.94E-04	2.57E-04	1.64E-04
	1.37E-02	1.27E-02	1.16E-02	1.04E-02	9.09E-03	7.80E-03	6.54E-03	5.35E-03	4.26E-03	3.31E-03	2.50E-03	1.85E-03	1.33E-03	9.40E-04	6.49E-04	4.40E-04	2.93E-04
	1.24E-02	1.19E-02	1.13E-02	1.06E-02	9.65E-03	8.62E-03	7.52E-03	6.40E-03	5.31E-03	4.29E-03	3.38E-03	2.60E-03	1.95E-03	1.43E-03	1.03E-03	7.26E-04	5.04E-04
	1.07E-02	1.08E-02	1.07E-02	1.04E-02	9.85E-03	9.16E-03	8.31E-03	7.36E-03	6.36E-03	5.35E-03	4.38E-03	3.51E-03	2.74E-03	2.09E-03	1.57E-03	1.15E-03	8.30E-04
	8.97E-03	9.39E-03	9.66E-03	9.76E-03	9.65E-03	9.34E-03	8.83E-03	8.14E-03	7.31E-03	6.40E-03	5.46E-03	4.55E-03	3.70E-03	2.94E-03	2.29E-03	1.75E-03	1.32E-03
	7.20E-03	7.84E-03	8.40E-03	8.83E-03	9.09E-03	9.16E-03	9.01E-03	8.64E-03	8.08E-03	7.36E-03	6.54E-03	5.67E-03	4.79E-03	3.97E-03	3.22E-03	2.56E-03	2.00E-03
	5.55E-03	6.29E-03	7.01E-03	7.67E-03	8.23E-03	8.62E-03	8.83E-03	8.82E-03	8.58E-03	8.14E-03	7.52E-03	6.78E-03	5.97E-03	5.14E-03	4.34E-03	3.59E-03	2.93E-03
	4.11E-03	4.85E-03	5.63E-03	6.41E-03	7.15E-03	7.80E-03	8.31E-03	8.64E-03	8.75E-03	8.64E-03	8.31E-03	7.80E-03	7.15E-03	6.41E-03	5.63E-03	4.85E-03	4.11E-03
	2.93E-03	3.59E-03	4.34E-03	5.14E-03	5.97E-03	6.78E-03	7.52E-03	8.14E-03	8.58E-03	8.82E-03	8.83E-03	8.62E-03	8.23E-03	7.67E-03	7.01E-03	6.29E-03	5.55E-03
	2.00E-03	2.56E-03	3.22E-03	3.97E-03	4.79E-03	5.67E-03	6.54E-03	7.36E-03	8.08E-03	8.64E-03	9.01E-03	9.16E-03	9.09E-03	8.83E-03	8.40E-03	7.84E-03	7.20E-03
	1.32E-03	1.75E-03	2.29E-03	2.94E-03	3.70E-03	4.55E-03	5.46E-03	6.40E-03	7.31E-03	8.14E-03	8.83E-03	9.34E-03	9.65E-03	9.76E-03	9.66E-03	9.39E-03	8.97E-03
	8.30E-04	1.15E-03	1.57E-03	2.09E-03	2.74E-03	3.51E-03	4.38E-03	5.35E-03	6.36E-03	7.36E-03	8.31E-03	9.16E-03	9.85E-03	1.04E-02	1.07E-02	1.08E-02	1.07E-02
	5.04E-04	7.26E-04	1.03E-03	1.43E-03	1.95E-03	2.60E-03	3.38E-03	4.29E-03	5.31E-03	6.40E-03	7.52E-03	8.62E-03	9.65E-03	1.06E-02	1.13E-02	1.19E-02	1.24E-02
	2.93E-04	4.40E-04	6.49E-04	9.40E-04	1.33E-03	1.85E-03	2.50E-03	3.31E-03	4.26E-03	5.35E-03	6.54E-03	7.80E-03	9.09E-03	1.04E-02	1.16E-02	1.27E-02	1.37E-02
	1.64E-04	2.57E-04	3.94E-04	5.93E-04	8.76E-04	1.26E-03	1.78E-03	2.45E-03	3.29E-03	4.29E-03	5.46E-03	6.78E-03	8.23E-03	9.76E-03	1.13E-02	1.29E-02	1.45E-02
	8.84E-05	1.44E-04	2.29E-04	3.60E-04	5.53E-04	8.31E-04	1.22E-03	1.74E-03	2.43E-03	3.31E-03	4.38E-03	5.67E-03	7.15E-03	8.83E-03	1.07E-02	1.27E-02	1.48E-02

Table 4-S. *Input modal composition mass fractions (by columns) in the Aitken mode and composition standard deviation for involatile core of 90%.*

n-alkanes $C_nH_{(2n+2)}$ n	Chickos&Lipkind 2008	EPI Suite	A) Nannoolal et al 2008 boiling point			B) Myrdal and Yalkowsky 1997 boiling point			Co) Compernolle et al 2011 for all boiling points
			a	b	c	a	b	c	
16		9.29E-001	2.87E-001	6.63E-001	5.38E-001	1.39E-001	3.46E-001	2.75E-001	3.05E-001
17		4.32E-001	6.85E-002	2.45E-001	2.06E-001	3.14E-002	1.24E-001	1.03E-001	9.98E-002
18		1.95E-001	1.54E-002	9.22E-002	7.91E-002	6.74E-003	4.55E-002	3.86E-002	3.27E-002
19		8.97E-002	3.23E-003	3.54E-002	3.04E-002	1.38E-003	1.73E-002	1.47E-002	1.07E-002
20		4.13E-002	6.33E-004	1.39E-002	1.17E-002	2.70E-004	6.76E-003	5.61E-003	3.50E-003
21	6.93E-004	1.89E-002	1.16E-004	5.60E-003	4.47E-003	5.03E-005	2.73E-003	2.16E-003	1.15E-003
22	2.09E-004	9.23E-003	1.97E-005	2.26E-003	1.71E-003	8.94E-006	1.11E-003	8.35E-004	3.75E-004
23	6.95E-005	4.73E-003	3.10E-006	8.86E-004	6.52E-004	1.52E-006	4.45E-004	3.25E-004	1.23E-004
24	2.31E-005	2.26E-003	4.50E-007	3.39E-004	2.48E-004	2.46E-007	1.75E-004	1.27E-004	4.01E-005
25	8.51E-006	1.28E-002	6.01E-008	1.26E-004	9.38E-005	3.81E-008	6.71E-005	4.97E-005	1.31E-005
26	2.83E-006	7.02E-004	7.37E-009	4.58E-005	3.53E-005	5.64E-009	2.53E-005	1.95E-005	4.30E-006
27	1.15E-006	1.31E-004	8.25E-010	1.61E-005	1.32E-005	7.97E-010	9.36E-006	7.68E-006	1.41E-006
28	3.14E-007	2.06E-004	8.40E-011	5.53E-006	4.94E-006	1.08E-010	3.39E-006	3.03E-006	4.61E-007
29	1.05E-007	1.27E-004	7.74E-012	1.84E-006	1.83E-006	1.39E-011	1.20E-006	1.20E-006	1.51E-007
30	3.48E-008	7.49E-005	6.44E-013	5.96E-007	6.75E-007	1.72E-012	4.20E-007	4.74E-007	4.93E-008
31	1.16E-008	4.54E-005	4.81E-014	1.87E-007	2.47E-007	2.03E-013	1.43E-007	1.88E-007	1.61E-008
32	3.49E-009	2.66E-005	3.20E-015	5.70E-008	9.01E-008	2.29E-014	4.80E-008	7.43E-008	5.28E-009

Table 5-S. *Vapour pressure data at 298 K from different sources corresponding to Figure 2 in the main manuscript. a, b, and c refer to the boiling point of Joback and Reid (1987), Stein and Brown (1994) and Nannoolal et al. (2004), respectively. A-a, B-c and Co are used in this study.*

compound	vapour
$C_{16}H_{34}$	6.42 (3.62)
$C_{17}H_{36}$	9.32 (4.31)
$C_{18}H_{38}$	9.36 (4.41)
$C_{19}H_{40}$	9.74 (4.09)
$C_{20}H_{42}$	8.35 (3.59)
$C_{21}H_{44}$	6.20 (3.06)
$C_{22}H_{46}$	3.97 (1.98)
$C_{23}H_{48}$	2.32 (1.25)
$C_{24}H_{50}$	1.59 (1.79)
$C_{25}H_{52}$	1.20 (0.52)
$C_{26}H_{54}$	1.00 (0.50)
$C_{27}H_{56}$	1.28 (0.53)
$C_{28}H_{58}$	1.03 (0.53)
$C_{29}H_{60}$	1.24 (0.53)
$C_{30}H_{62}$	0.80 (0.38)
$C_{31}H_{64}$	0.77 (0.30)
$C_{32}H_{66}$	0.42 (0.18)

Table 6-S. *Gas-phase concentrations used in the model. Numbers in parenthesis show the standard deviation of the measurements. Unit, ng* m^{-3}.