Support information

The Effect of Temperature on the Surface Energetic Properties of Carbon Fibers using Inverse Gas Chromatography

Tayssir Hamieh[1,2]

[1]Faculty of Science and Engineering, Maastricht University, P.O. Box 616, 6200 MD Maastricht, Netherlands, E-mail: t.hamieh@maastrichtuniversity.nl
[2]Laboratory of Materials, Catalysis, Environment and Analytical Methods Laboratory (MCEMA), Faculty of Sciences, Lebanese University, 1533, Hadath, Lebanon

Surface area of n-alkanes

Knowing that the surface area of organic solvents depends on the chosen molecular model, one presented on Table S1, the values corresponding to the different models.

Table S1. Surface areas of various molecules (in $Å^2$) given by the various models of Van der Waals (VDW), Redlich-Kwong (R-K), Kiselev, geometric, cylindrical or spherical models.

Molecules	VDW	Kiselev	Cylindrical	R-K	Spherical	Geometric
C_6H_{14}	52.7	51.5	45.5	41.3	39.6	40.7
C_7H_{16}	59.2	57	51.8	46.4	42.7	48.5
C_8H_{18}	64.9	63	58.1	50.8	45.7	56.2
C_9H_{20}	69.6	69	64.4	54.5	48.7	64.0

Expressions of the dispersive components of the surface energy of n-alkanes

The general expressions $\gamma_{l\,X}^{d}\,(T)$ of the London dispersive component of the surface energy of organic molecule (denoted X) can be given by a linear relation in the usual domain of the temperature with an excellent linear regression coefficient approaching 1.0000

$$\gamma_{l\,X}^{d}\,(T) = \varepsilon_X T + \gamma_{l\,X}^{d}(0K);\ \varepsilon_X = \frac{d\gamma_{l\,X}^{d}}{dT} \qquad (1)$$

Where ε_X is the surface entropy of the molecule X and $\gamma_{l\,X}^{d}(0K)$ the London dispersive surface energy of the solvent extrapolated to 0K. ε_X and $\gamma_{l\,X}^{d}(0K)$ are constants only depending on the solvent nature.

On Table S2, one gave the two parameters ε_X and $\gamma_{l\,X}^{d}(0K)$ of the straight lines representing

$\gamma_{lX}^{d}(T)$ for the different used n-alkanes. The values on Table 1 proved that the slope of the linear equations is negative showing a decrease of the London dispersive surface energy when the temperature increases.

Table S2. Values of the surface entropy $\varepsilon_X\ (in\ mJ/(K \times m^2))$ and $\gamma_{lX}^{d}(0K)(in\ mJ/m^2)$ of the n-alkanes

Molecule X	ε_X	$\gamma_{lX}^{d}(0K)$
C5	-0.110	48.33
C6	-0.102	48.34
C7	-0.098	48.85
C8	-0.095	49.48
C9	-0.093	50.26
C10	-0.092	50.79

Characteristics of the used polar molecules

Different polar molecules were used in this study. Their characteristics are presented on Table S3.

Table S3. Normalized donor and acceptor numbers of some polar molecules.

polar probe	DN'	AN'	DN'/AN'	Character
CCl_4	0	2.3	0	Acid
$CHCl_3$	0	18.7	0.00	Higher acidity
CH_2Cl_2	3	13.5	0.22	Acid
Benzene	0.25	0.6	0.42	Weaker amphoteric
Acetone	42.5	8.7	4.89	Higher amphoteric
Ethyl acetate	42.75	5.3	8.07	Base
Diethyl ether	48	4.9	9.80	Base
THF	50	1.9	26.32	Higher basicity

Retention volume of the different molecules adsorbed on carbon fibers

Table S4. Values of $RTlnVn$ (in kJ/mol) of the various polar solvents adsorbed on untreated carbon fibers (a) as a function of the temperature.

T(K)	313.15	323.15	333.15	343.15	353.15	363.15	373.15
C6	0.591	0.388	0.185	-0.018	-0.221	-0.424	-0.627
C7	3.859	3.589	3.319	3.049	2.779	2.509	2.239
C8	6.487	6.244	6.001	5.758	5.515	5.272	5.029
C9	9.917	9.494	9.101	8.686	8.285	7.984	7.734

CCl4	1.830	1.760	1.690	1.626	1.564	1.500	1.442
CH2Cl2	-2.639	-2.911	-3.212	-3.517	-3.851	-4.279	-4.787
CHCl3	11.181	10.463	9.653	8.741	7.642	6.137	3.682
Ether	-1.970	-2.305	-2.668	-3.019	-3.389	-3.848	-4.362
THF	5.562	5.107	4.651	4.197	3.743	3.282	2.820
Benzene	5.709	5.441	5.183	4.919	4.659	4.428	4.213
Ethyl acetate	5.326	5.092	4.860	4.634	4.412	4.191	3.982
Acetone	1.539	1.308	1.065	0.841	0.616	0.348	0.071

Table S5. Values of $RTlnVn$ (in kJ/mol) of the various polar solvents adsorbed on oxidized carbon fibers (b) as a function of the temperature.

T(K)	**313.15**	**323.15**	**333.15**	**343.15**	**353.15**	**363.15**	**373.15**
C6	1.211	1.143	1.061	0.979	0.897	0.815	0.733
C7	4.409	4.139	3.869	3.599	3.329	3.059	2.789
C8	7.192	6.814	6.436	6.058	5.680	5.302	4.924
C9	10.445	10.107	9.769	9.431	9.093	8.755	8.417
CCl4	3.505	3.427	3.341	3.256	3.173	3.090	3.009
CH2Cl2	4.441	4.238	4.035	3.832	3.629	3.426	3.223
CHCl3	9.763	9.484	9.205	8.926	8.647	8.368	8.089
Ether	3.941	3.738	3.535	3.332	3.129	2.926	2.723
THF	11.359	10.873	10.379	9.886	9.394	8.902	8.411
Benzene	8.182	7.919	7.652	7.386	7.120	6.855	6.590
Ethyl acetate	9.662	9.432	9.202	8.972	8.742	8.512	8.282
Acetone	9.379	9.082	8.785	8.488	8.191	7.894	7.597

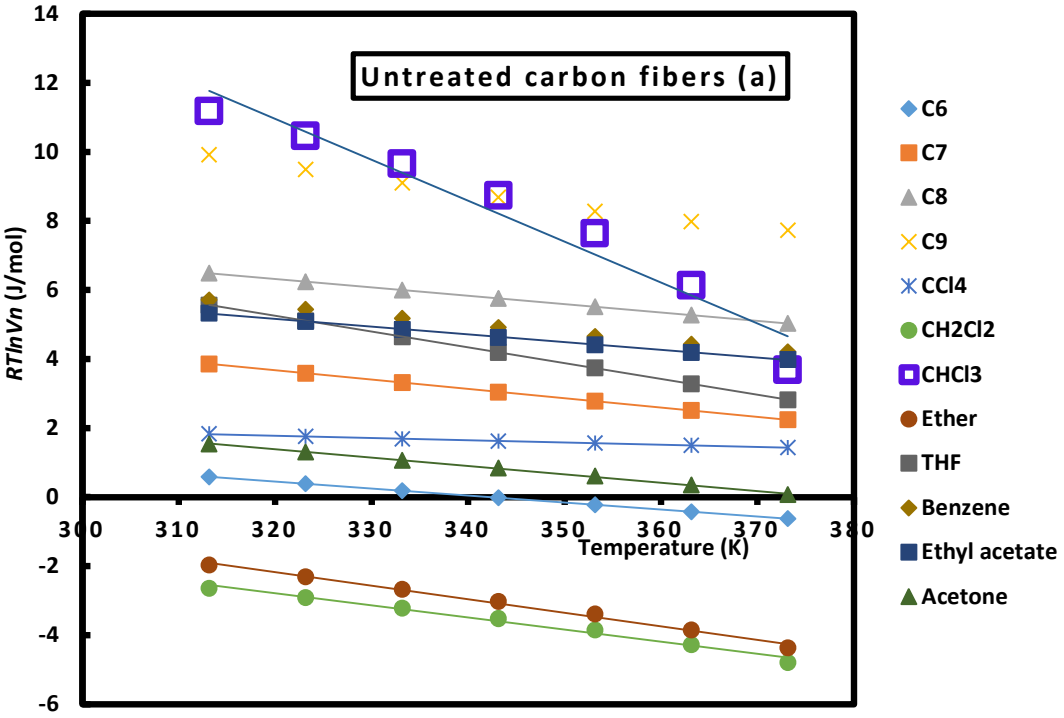


Figure S1. Variations of $RTlnVn$ of the various solvents adsorbed on untreated carbon fibers (a) as a function of the temperature.

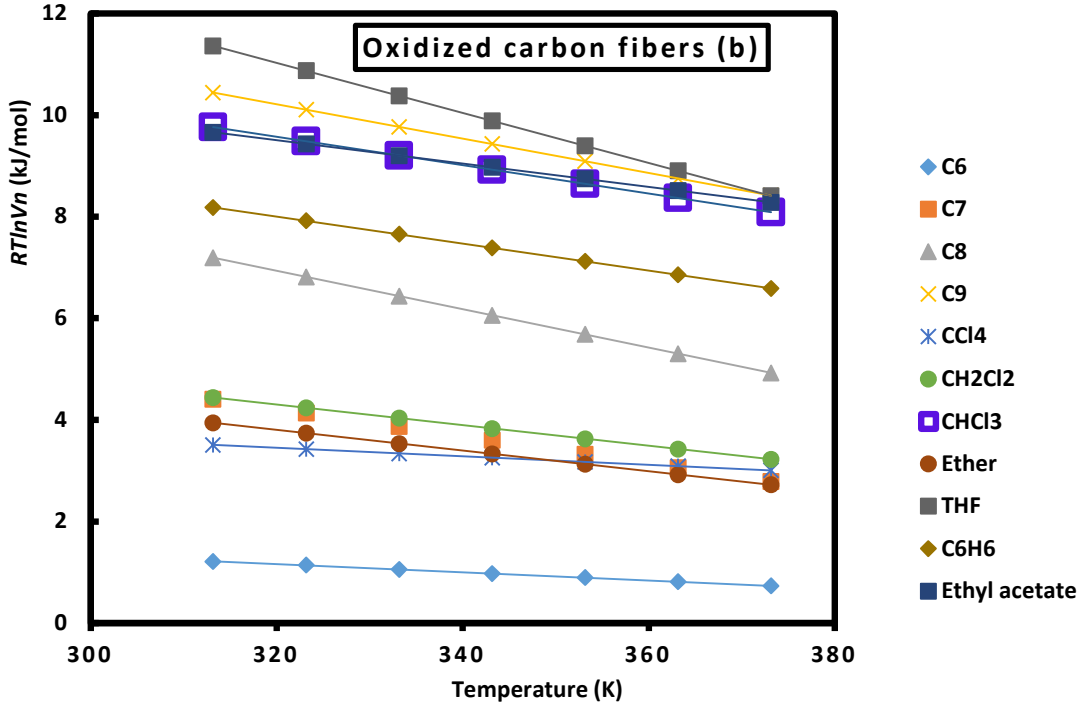


Figure S2. Variations of $RTlnVn$ of the various solvents adsorbed on oxidized carbon fibers (b) as a function of the temperature.

Table S6. Values of ($\Delta G_a^{sp}(T)$) (in kJ/mol) of the various polar solvents adsorbed untreated carbon fibers (a) as a function of the temperature by using the various models and IGC methods.

ΔG_a^{sp} (T) (in kJ/mol)	Kiselev							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	0.824	0.574	11.836	3.453	3.938	0.514	4.275	5.405
323.15	0.816	0.554	12.022	3.170	3.666	0.506	4.050	5.052
333.15	0.808	0.534	12.208	2.887	3.394	0.498	3.825	4.699
343.15	0.800	0.514	12.394	2.604	3.122	0.490	3.600	4.346
353.15	0.792	0.494	12.580	2.321	2.850	0.482	3.375	3.993
363.15	0.784	0.474	12.766	2.038	2.578	0.474	3.150	3.640
373.15	0.776	0.454	12.952	1.755	2.306	0.466	2.925	3.287

ΔG_a^{sp} (T) (in kJ/mol)	Spherical							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	1.586	3.200	15.423	3.028	7.271	5.282	6.767	7.380
323.15	1.502	3.075	15.510	2.816	6.824	5.043	6.380	6.873
333.15	1.423	2.959	15.607	2.606	6.386	4.818	6.002	6.373
343.15	1.343	2.836	15.694	2.401	5.940	4.581	5.620	5.871
353.15	1.264	2.715	15.785	2.199	5.495	4.347	5.241	5.371
363.15	1.191	2.616	15.918	2.002	5.076	4.151	4.882	4.885
373.15	1.119	2.526	16.107	1.813	4.664	3.967	4.530	4.404

ΔG_a^{sp} (T) (in kJ/mol)	Geometric							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	5.857	3.791	16.625	0.428	4.716	3.618	5.976	3.436
323.15	5.722	3.494	16.108	0.266	4.421	3.510	5.758	3.217
333.15	5.600	3.194	15.552	0.098	4.130	3.411	5.546	2.994
343.15	5.464	2.873	14.912	-0.063	3.836	3.303	5.328	2.775
353.15	5.331	2.538	14.162	-0.228	3.542	3.196	5.111	2.554
363.15	5.242	2.198	13.211	-0.416	3.255	3.116	4.911	2.321
373.15	5.172	1.828	11.682	-0.615	2.971	3.047	4.720	2.085

ΔG_a^{sp} (T) (in kJ/mol)	VDW							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
297.95	1.400	1.939	15.071	2.185	7.265	5.817	5.652	5.958
307.85	1.364	1.846	14.993	1.992	6.844	5.588	5.369	5.577
313.45	1.330	1.756	14.909	1.796	6.430	5.373	5.089	5.196
323.75	1.294	1.660	14.800	1.606	6.006	5.142	4.806	4.813
333.45	1.258	1.564	14.664	1.417	5.585	4.916	4.523	4.431
342.65	1.225	1.471	14.489	1.219	5.186	4.729	4.250	4.050

353.25	1.193	1.375	14.176	1.022	4.793	4.556	3.980	3.667

ΔG_a^{sp} (T) (in kJ/mol)	Redlich-Kwong (R-K)							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	1.445	2.009	15.125	2.234	7.314	5.825	5.683	5.991
323.15	1.407	1.912	15.045	2.038	6.890	5.595	5.398	5.607
333.15	1.371	1.818	14.959	1.840	6.474	5.379	5.116	5.224
343.15	1.332	1.718	14.846	1.647	6.048	5.148	4.831	4.840
353.15	1.294	1.618	14.707	1.455	5.624	4.920	4.546	4.455
363.15	1.259	1.521	14.530	1.255	5.222	4.732	4.271	4.071
373.15	1.225	1.422	14.215	1.056	4.828	4.560	4.000	3.688

ΔG_a^{sp} (T) (in kJ/mol)	Cylindrical							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	1.312	5.054	17.423	0.460	2.543	-1.321	4.516	2.558
323.15	1.304	4.717	16.978	0.334	2.334	-1.254	4.308	2.340
333.15	1.296	4.383	16.507	0.201	2.121	-1.192	4.100	2.115
343.15	1.288	4.027	15.967	0.080	1.913	-1.124	3.891	1.897
353.15	1.278	3.659	15.344	-0.043	1.703	-1.059	3.681	1.676
363.15	1.273	3.303	14.581	-0.184	1.483	-1.008	3.474	1.433
373.15	1.271	2.926	13.383	-0.327	1.260	-0.961	3.269	1.183

ΔG_a^{sp} (T) (in kJ/mol)	Hamieh model							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	1.224	1.274	10.200	2.312	7.316	0.912	10.622	4.796
323.15	1.216	1.254	10.674	2.011	7.165	0.906	10.246	4.575
333.15	1.208	1.234	11.161	1.689	7.037	0.900	9.881	4.345
343.15	1.200	1.214	11.670	1.346	6.913	0.894	9.489	4.104
353.15	1.192	1.194	12.212	0.976	6.811	0.888	9.094	3.853
363.15	1.184	1.174	12.820	0.561	6.776	0.882	8.746	3.590
373.15	1.176	1.154	13.621	0.098	6.802	0.876	8.411	3.317

ΔG_a^{sp} (T) (in kJ/mol)	Topological index							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	8.19	7.28	19.17	1.22	8.69	4.32	6.459	8.296
323.15	8.16	6.98	18.46	1.00	8.35	4.26	6.379	8.103
333.15	8.16	6.69	17.69	0.76	8.02	4.21	6.311	7.924
343.15	8.15	6.37	16.80	0.53	7.69	4.15	6.241	7.744
353.15	8.16	6.03	15.74	0.28	7.36	4.10	6.181	7.577
363.15	8.25	5.73	14.37	0.00	7.08	4.09	6.159	7.458
373.15	8.38	5.40	12.11	-0.30	6.82	4.10	6.167	7.378

ΔG_a^{sp} (T) (in kJ/mol)	Deformation polarizability							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	9.56	-3.82	14.46	2.70	11.62	6.76	8.321	10.378
323.15	9.50	-3.89	13.84	2.44	11.21	6.64	8.202	10.140
333.15	9.48	-3.98	13.16	2.18	10.84	6.55	8.102	9.926
343.15	9.44	-4.09	12.36	1.91	10.44	6.45	7.996	9.705
353.15	9.42	-4.22	11.39	1.64	10.06	6.35	7.900	9.498
363.15	9.50	-4.42	10.06	1.35	9.75	6.32	7.863	9.362
373.15	9.63	-4.71	7.82	1.04	9.49	6.32	7.863	9.275

ΔG_a^{sp} (T) (in kJ/mol)	Vapor pressure							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	0.467	-2.552	13.401	0.756	5.352	3.914	5.762	2.085
323.15	0.588	-2.639	12.886	0.600	5.039	3.868	5.782	2.079
333.15	0.714	-2.747	12.292	0.430	4.732	3.834	5.808	2.071
343.15	0.844	-2.865	11.582	0.257	4.424	3.791	5.831	2.076
353.15	0.980	-3.009	10.691	0.070	4.119	3.755	5.858	2.083
363.15	1.125	-3.221	9.440	-0.153	3.830	3.754	5.917	2.083
373.15	1.284	-3.499	7.267	-0.405	3.552	3.775	6.003	2.094

ΔG_a^{sp} (T) (in kJ/mol)	Boiling point							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	0.45	0.11	10.53	1.26	5.50	3.95	3.905	2.447
323.15	0.60	-0.04	10.01	1.04	5.24	3.91	3.886	2.383
333.15	0.72	-0.22	9.38	0.79	4.95	3.84	3.844	2.291
343.15	0.86	-0.40	8.66	0.55	4.67	3.80	3.827	2.230
353.15	1.03	-0.58	7.78	0.33	4.43	3.77	3.836	2.192
363.15	1.16	-0.85	6.46	0.02	4.15	3.74	3.808	2.097
373.15	1.35	-1.12	4.25	-0.26	3.93	3.77	3.848	2.060

ΔG_a^{sp} (T) (in kJ/mol)	ΔHvap							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	0.681	-2.687	10.827	0.120	4.658	3.686	2.588	1.062
323.15	0.811	-2.782	10.292	-0.081	4.398	3.637	2.587	1.018
333.15	0.948	-2.896	9.676	-0.295	4.144	3.601	2.590	0.970
343.15	1.083	-3.023	8.946	-0.511	3.885	3.553	2.595	0.932
353.15	1.226	-3.173	8.038	-0.737	3.630	3.514	2.606	0.898
363.15	1.381	-3.391	6.745	-1.004	3.387	3.510	2.620	0.844
373.15	1.550	-3.677	4.514	-1.304	3.151	3.525	2.643	0.792

ΔG_a^{sp} (T) (in kJ/mol)	ΔHvap (T)

T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	0.549	-2.456	10.544	-0.042	4.386	4.787	4.404	-0.502
323.15	0.408	-2.667	9.600	-0.690	3.778	4.664	4.315	-0.255
333.15	0.269	-2.923	8.579	-1.357	3.177	4.532	4.210	-0.062
343.15	0.148	-3.194	7.476	-2.003	2.599	4.383	4.099	0.114
353.15	0.044	-3.500	6.214	-2.643	2.041	4.230	3.983	0.254
363.15	-0.052	-3.890	4.566	-3.334	1.492	4.105	3.869	0.326
373.15	-0.128	-4.356	1.994	-4.050	0.962	3.996	3.765	0.369

Table S7. Values of ($\Delta G_a^{sp}(T)$) (in kJ/mol) of the various polar solvents oxidized carbon fibers (b) as a function of the temperature by using the various models and IGC methods.

ΔG_a^{sp} (T) (in kJ/mol)	Kiselev							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	1.883	7.019	9.793	8.720	9.121	2.387	7.994	12.608
323.15	1.809	6.968	10.334	8.452	8.764	2.362	7.716	12.088
333.15	1.735	6.941	10.949	8.205	8.407	2.337	7.446	11.582
343.15	1.661	6.924	11.654	7.962	8.050	2.312	7.175	11.073
353.15	1.587	6.922	12.505	7.725	7.693	2.287	6.903	10.562
363.15	1.513	6.941	13.630	7.496	7.336	2.262	6.631	10.049
373.15	1.439	6.989	15.494	7.280	6.979	2.237	6.358	9.533

ΔG_a^{sp} (T) (in kJ/mol)	Spherical							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	2.641	9.635	13.367	8.298	12.441	7.136	10.477	14.576
323.15	2.483	9.450	13.771	8.097	11.875	6.835	10.011	13.879
333.15	2.329	9.294	14.251	7.920	11.317	6.544	9.562	13.203
343.15	2.177	9.147	14.819	7.748	10.758	6.253	9.115	12.528
353.15	2.028	9.015	15.533	7.585	10.201	5.964	8.671	11.855
363.15	1.881	8.904	16.525	7.434	9.645	5.676	8.231	11.184
373.15	1.737	8.823	18.289	7.299	9.090	5.389	7.794	10.515

ΔG_a^{sp} (T) (in kJ/mol)	Geometric							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	6.894	10.221	14.562	5.706	9.894	5.477	9.687	10.647
323.15	6.648	9.868	14.366	5.587	9.508	5.326	9.401	10.278
333.15	6.407	9.535	14.210	5.485	9.124	5.177	9.124	9.920
343.15	6.164	9.205	14.088	5.388	8.739	5.027	8.844	9.558
353.15	5.919	8.877	14.020	5.298	8.355	4.877	8.561	9.194
363.15	5.670	8.555	14.053	5.216	7.969	4.725	8.275	8.826
373.15	5.417	8.240	14.359	5.147	7.583	4.571	7.984	8.454

ΔG_a^{sp} (T) (in kJ/mol)	VDW							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
2.457	8.382	13.018	7.461	12.436	7.669	9.367	13.163	5.958
2.343	8.232	13.254	7.279	11.890	7.370	9.010	12.595	5.577
2.231	8.107	13.557	7.117	11.349	7.076	8.665	12.043	5.196
2.121	7.992	13.935	6.962	10.809	6.785	8.320	11.491	4.813
2.011	7.891	14.433	6.815	10.269	6.492	7.976	10.938	4.431
1.900	7.808	15.158	6.677	9.727	6.198	7.630	10.383	4.050
1.792	7.754	16.503	6.556	9.187	5.905	7.287	9.828	3.667

ΔG_a^{sp} (T) (in kJ/mol)	R-K							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	2.502	8.451	13.072	7.509	12.485	7.677	9.397	13.195
323.15	2.386	8.297	13.305	7.324	11.936	7.377	9.039	12.625
333.15	2.271	8.168	13.606	7.160	11.393	7.083	8.692	12.071
343.15	2.158	8.049	13.980	7.002	10.849	6.790	8.344	11.516
353.15	2.045	7.943	14.475	6.851	10.306	6.496	7.997	10.960
363.15	1.933	7.857	15.198	6.712	9.763	6.203	7.651	10.405
373.15	1.821	7.796	16.539	6.586	9.218	5.908	7.304	9.846

ΔG_a^{sp} (T) (in kJ/mol)	Cylindrical							
T(K)	CCl4	CHCl3	CH2Cl2	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	2.368	11.481	15.358	5.739	7.731	0.560	8.234	9.774
323.15	2.289	11.074	15.223	5.652	7.449	0.626	7.969	9.412
333.15	2.209	10.690	15.138	5.584	7.164	0.689	7.712	9.061
343.15	2.129	10.311	15.100	5.522	6.881	0.753	7.454	8.707
353.15	2.049	9.937	15.137	5.468	6.598	0.818	7.193	8.351
363.15	1.967	9.572	15.317	5.425	6.315	0.883	6.932	7.993
373.15	1.884	9.219	15.879	5.397	6.032	0.948	6.668	7.631

ΔG_a^{sp} (T) (in kJ/mol)	Hamieh model							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	2.214	1.371	2.429	7.584	12.485	0.739	14.315	12.002
323.15	2.132	1.321	2.142	7.305	12.213	0.669	13.825	11.615
333.15	2.050	1.271	1.855	7.029	11.952	0.599	13.343	11.230
343.15	1.968	1.221	1.568	6.737	11.700	0.529	12.849	10.831
353.15	1.886	1.171	1.281	6.430	11.460	0.459	12.344	10.418
363.15	1.804	1.121	0.994	6.106	11.232	0.389	11.827	9.990
373.15	1.722	1.071	0.707	5.767	11.024	0.319	11.299	9.547

ΔG_a^{sp} (T) (in kJ/mol)	Topological index

T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	9.215	13.701	17.095	6.498	13.855	6.178	10.168	15.487
323.15	9.054	13.309	16.685	6.307	13.383	6.065	10.012	15.095
333.15	8.903	12.940	16.295	6.131	12.917	5.955	9.867	14.723
343.15	8.755	12.570	15.905	5.954	12.452	5.846	9.722	14.350
353.15	8.607	12.201	15.515	5.778	11.988	5.739	9.578	13.978
363.15	8.460	11.832	15.126	5.601	11.525	5.631	9.433	13.605
373.15	8.315	11.463	14.736	5.425	11.062	5.524	9.289	13.233

ΔG_a^{sp} (T) (in kJ/mol)	Deformation polarizability							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	10.578	2.646	12.402	7.965	16.769	8.604	12.023	17.560
323.15	10.375	2.585	12.131	7.729	16.208	8.416	11.810	17.106
333.15	10.185	2.533	11.876	7.510	15.658	8.236	11.612	16.673
343.15	9.998	2.482	11.622	7.292	15.110	8.059	11.415	16.242
353.15	9.811	2.430	11.367	7.073	14.563	7.881	11.216	15.809
363.15	9.625	2.379	11.112	6.854	14.015	7.703	11.018	15.377
373.15	9.441	2.328	10.857	6.636	13.469	7.527	10.821	14.945

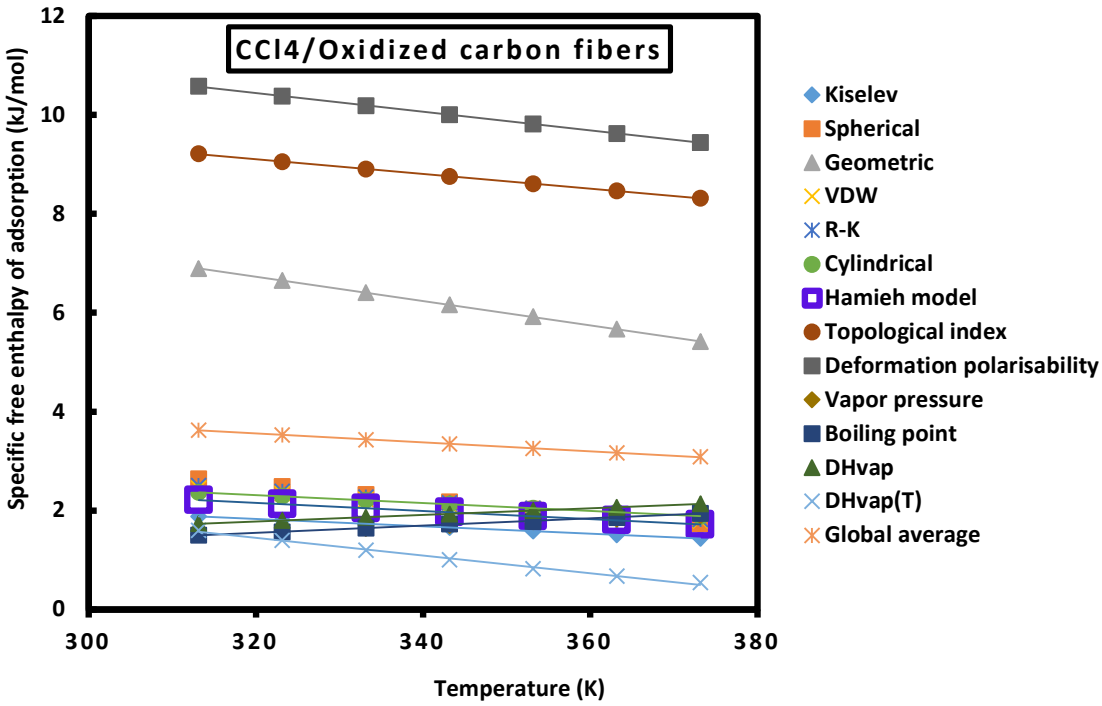
ΔG_a^{sp} (T) (in kJ/mol)	Vapor pressure							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	1.526	3.906	11.352	6.034	10.528	5.772	9.475	9.302
323.15	1.582	3.817	11.184	5.914	10.116	5.677	9.422	9.153
333.15	1.639	3.738	11.026	5.803	9.707	5.586	9.375	9.015
343.15	1.699	3.658	10.863	5.689	9.301	5.495	9.322	8.876
353.15	1.762	3.577	10.696	5.570	8.898	5.404	9.264	8.735
363.15	1.827	3.496	10.526	5.448	8.497	5.314	9.202	8.594
373.15	1.892	3.412	10.349	5.319	8.098	5.221	9.132	8.449

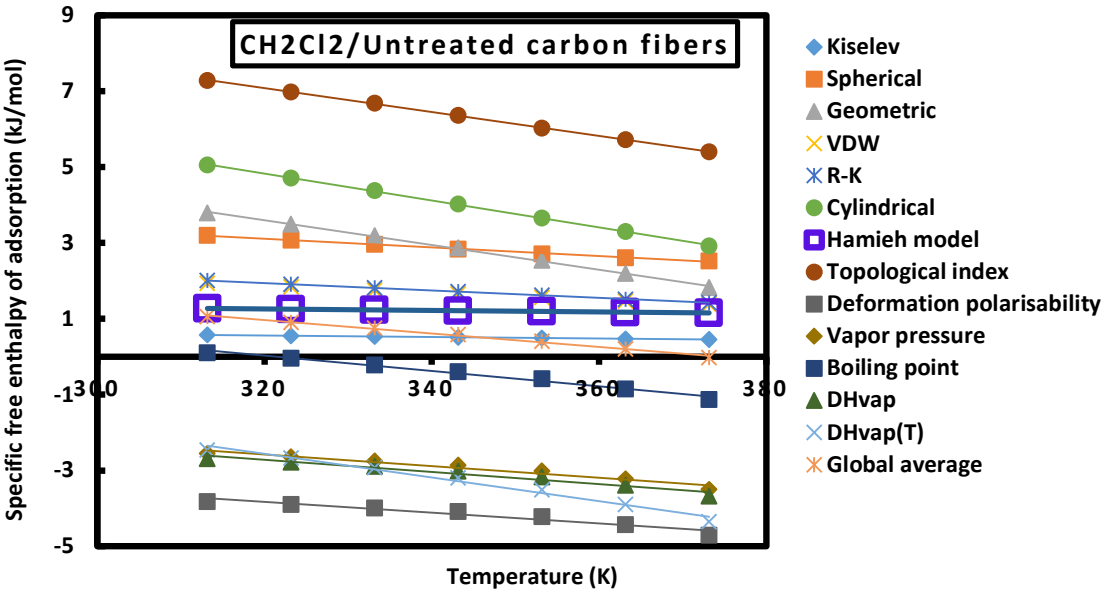
ΔG_a^{sp} (T) (in kJ/mol)	Boiling point							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	1.50	6.55	8.49	6.53	10.67	5.80	7.61629	9.65479
323.15	1.57	6.36	8.32	6.32	10.28	5.69	7.52697	9.42758
333.15	1.65	6.20	8.19	6.15	9.92	5.60	7.46463	9.22944
343.15	1.73	6.04	8.06	5.98	9.55	5.51	7.40329	9.03229
353.15	1.78	5.85	7.89	5.77	9.15	5.39	7.30593	8.80121
363.15	1.86	5.70	7.76	5.60	8.79	5.30	7.24459	8.60407
373.15	1.95	5.54	7.62	5.43	8.43	5.22	7.18225	8.40592

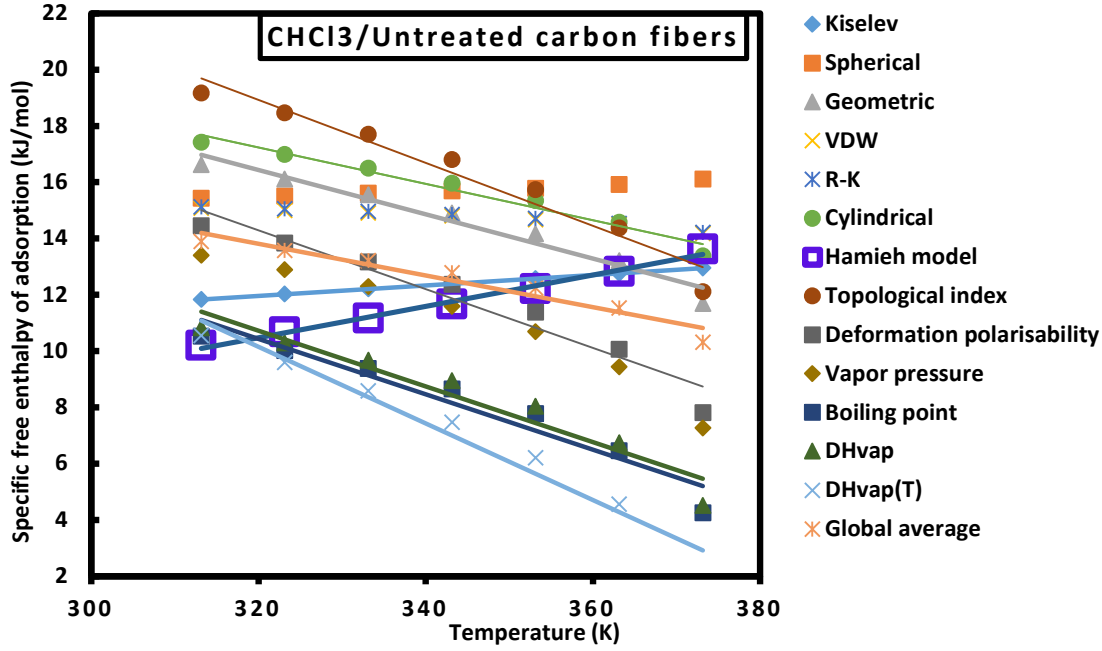
ΔG_a^{sp} (T) (in kJ/mol)	ΔHvap							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	1.73934	3.771	8.789	5.401	9.837	5.546	6.313	8.283

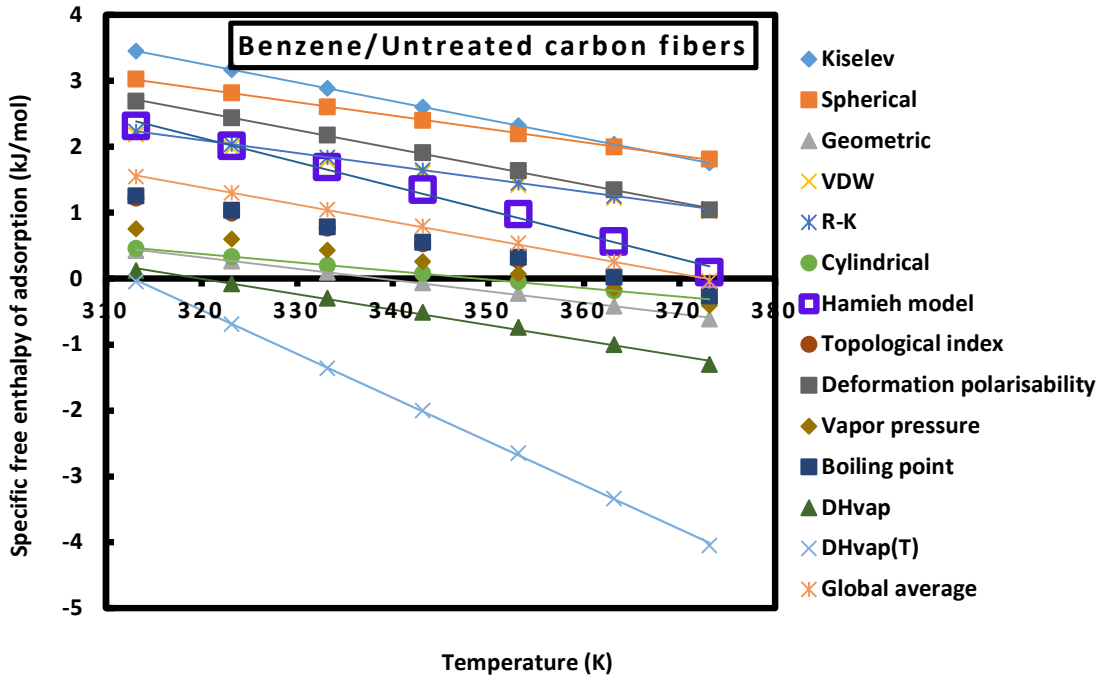
323.15	1.80209	3.676	8.627	5.242	9.484	5.449	6.272	8.107
333.15	1.86555	3.591	8.475	5.096	9.133	5.357	6.237	7.941
343.15	1.93425	3.510	8.326	4.953	8.786	5.270	6.206	7.778
353.15	1.99982	3.424	8.174	4.807	8.436	5.179	6.171	7.610
363.15	2.06732	3.340	8.022	4.661	8.088	5.088	6.136	7.444
373.15	2.14	3.255	7.870	4.515	7.740	4.998	6.102	7.278

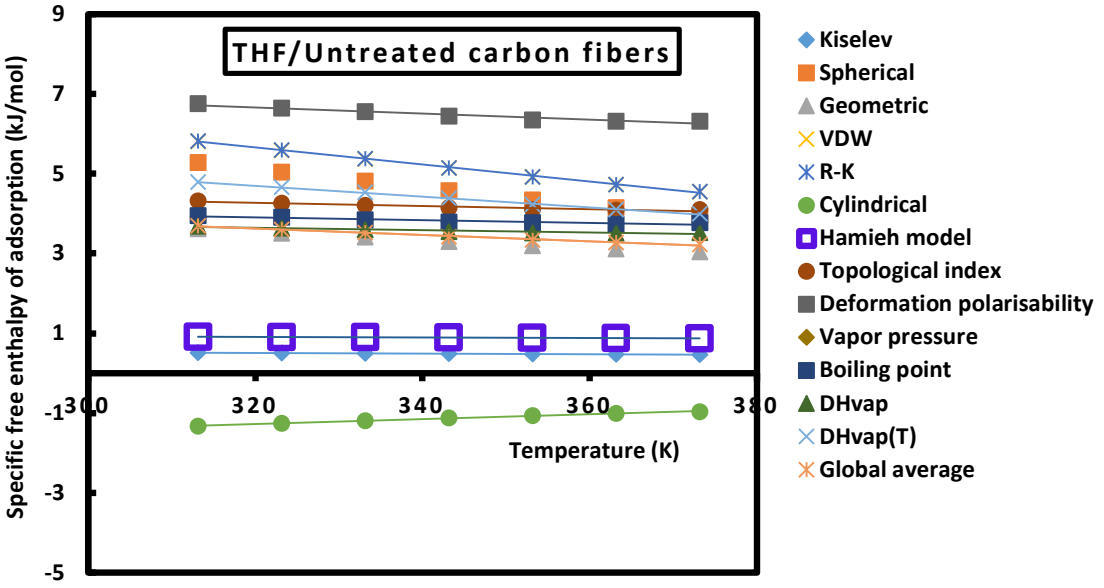
ΔG_a^{sp} (T) (in kJ/mol)	ΔHvap(T)							
T(K)	CCl4	CH2Cl2	CHCl3	Benzene	Diethyl ether	THF	Ethyl acetate	Acetone
313.15	1.60	4.00	8.50	5.23	9.56	6.64	8.118	6.722
323.15	1.40	3.79	7.94	4.64	8.87	6.46	7.976	6.852
333.15	1.20	3.56	7.40	4.05	8.19	6.26	7.809	6.929
343.15	1.00	3.30	6.88	3.47	7.52	6.03	7.621	6.955
353.15	0.83	3.04	6.39	2.91	6.88	5.80	7.418	6.931
363.15	0.67	2.76	5.93	2.38	6.27	5.55	7.206	6.861
373.15	0.55	2.50	5.52	1.89	5.70	5.30	6.994	6.755

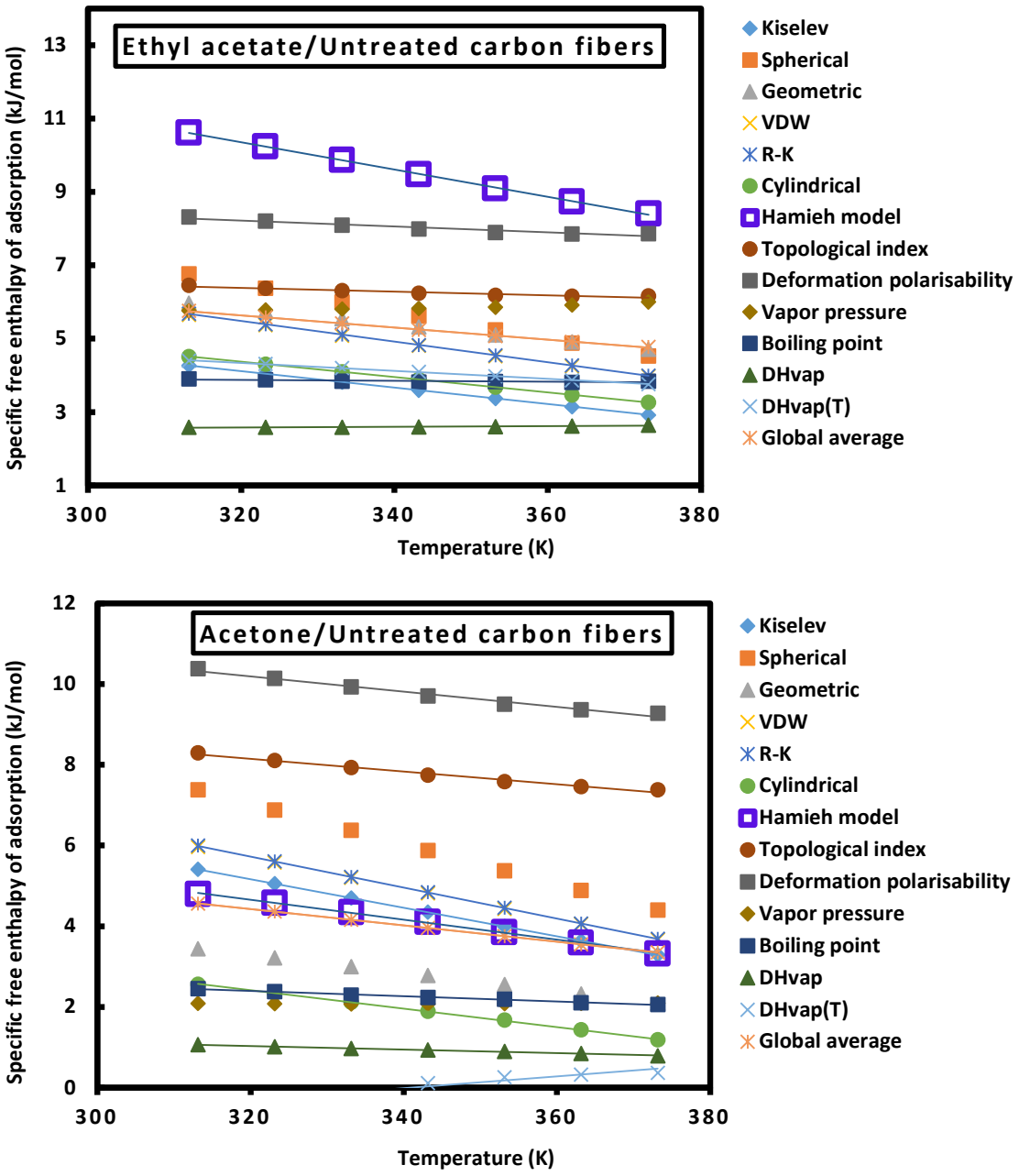



CH2Cl2/Untreated carbon fibers
Specific free enthalpy of adsorption (kJ/mol)
Temperature (K)
Kiselev
Spherical
Geometric
VDW
R-K
Cylindrical
Hamieh model
Topological index
Deformation polarisability
Vapor pressure
Boiling point
DHvap
DHvap(T)
Global average

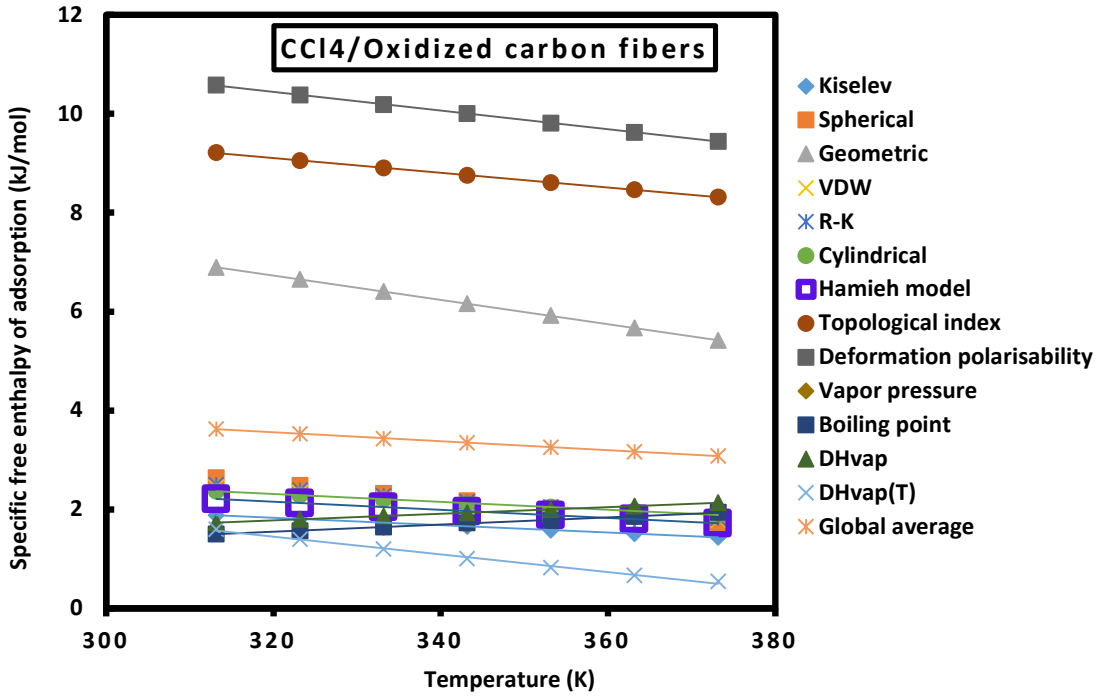

CHCl3/Untreated carbon fibers
Specific free enthalpy of adsorption (kJ/mol)
Temperature (K)
Kiselev
Spherical
Geometric
VDW
R-K
Cylindrical
Hamieh model
Topological index
Deformation polarisability
Vapor pressure
Boiling point
DHvap
DHvap(T)
Global average

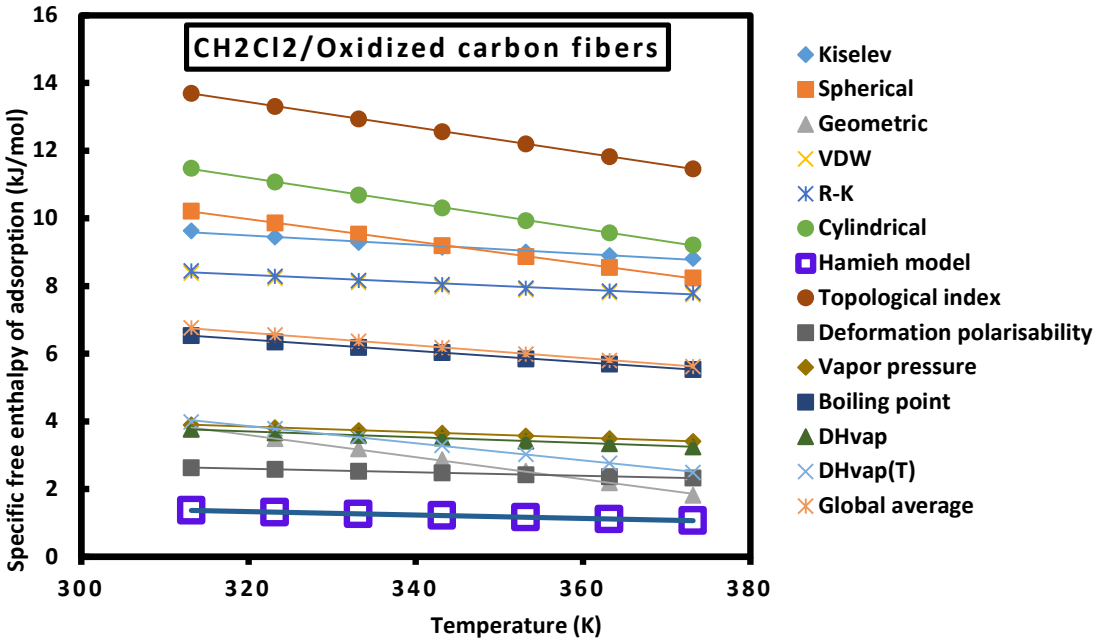

Benzene/Untreated carbon fibers
Specific free enthalpy of adsorption (kJ/mol)
Temperature (K)
Kiselev
Spherical
Geometric
VDW
R-K
Cylindrical
Hamieh model
Topological index
Deformation polarisability
Vapor pressure
Boiling point
DHvap
DHvap(T)
Global average

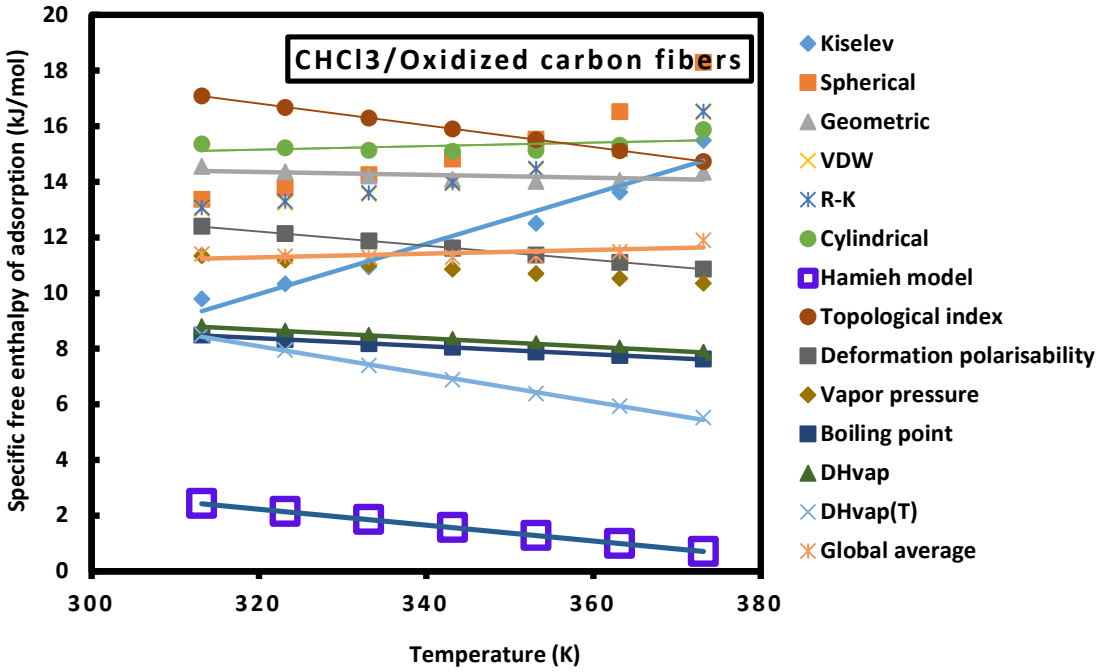

THF/Untreated carbon fibers
Specific free enthalpy of adsorption (kJ/mol)
Temperature (K)
Kiselev
Spherical
Geometric
VDW
R-K
Cylindrical
Hamieh model
Topological index
Deformation polarisability
Vapor pressure
Boiling point
DHvap
DHvap(T)
Global average

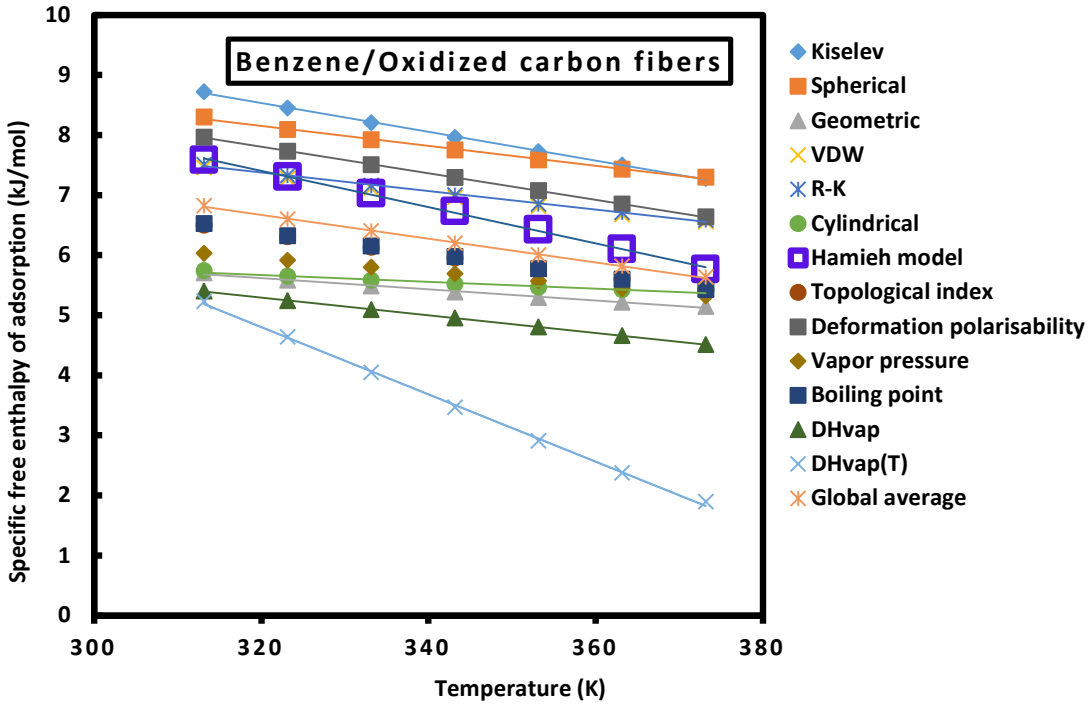


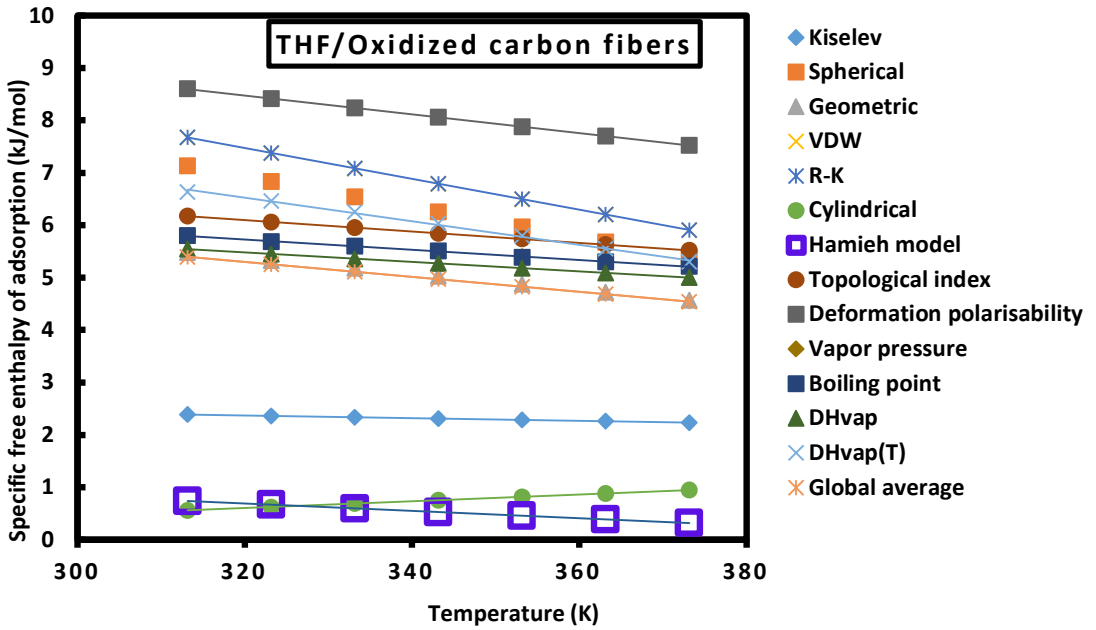
Figures S3. Variations of ΔG_a^{sp} of the various solvents adsorbed on untreated carbon fibers as a function of the temperature for the different models and chromatographic methods.

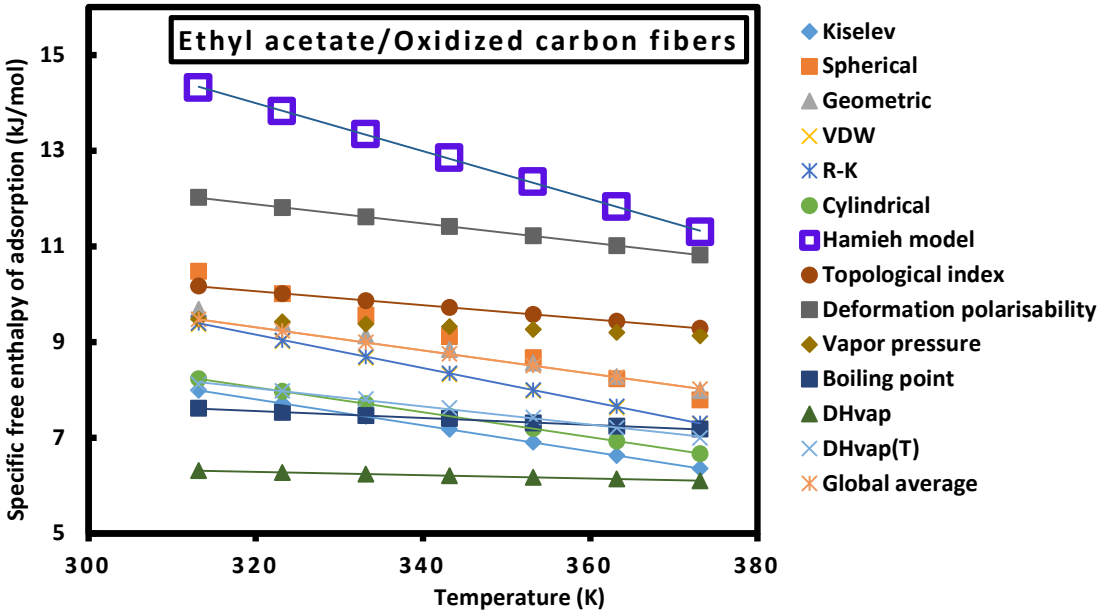

CCl4/Oxidized carbon fibers
Specific free enthalpy of adsorption (kJ/mol)
Temperature (K)
0
2
4
6
8
10
12
300
320
340
360
380
Kiselev
Spherical
Geometric
VDW
R-K
Cylindrical
Hamieh model
Topological index
Deformation polarisability
Vapor pressure
Boiling point
DHvap
DHvap(T)
Global average

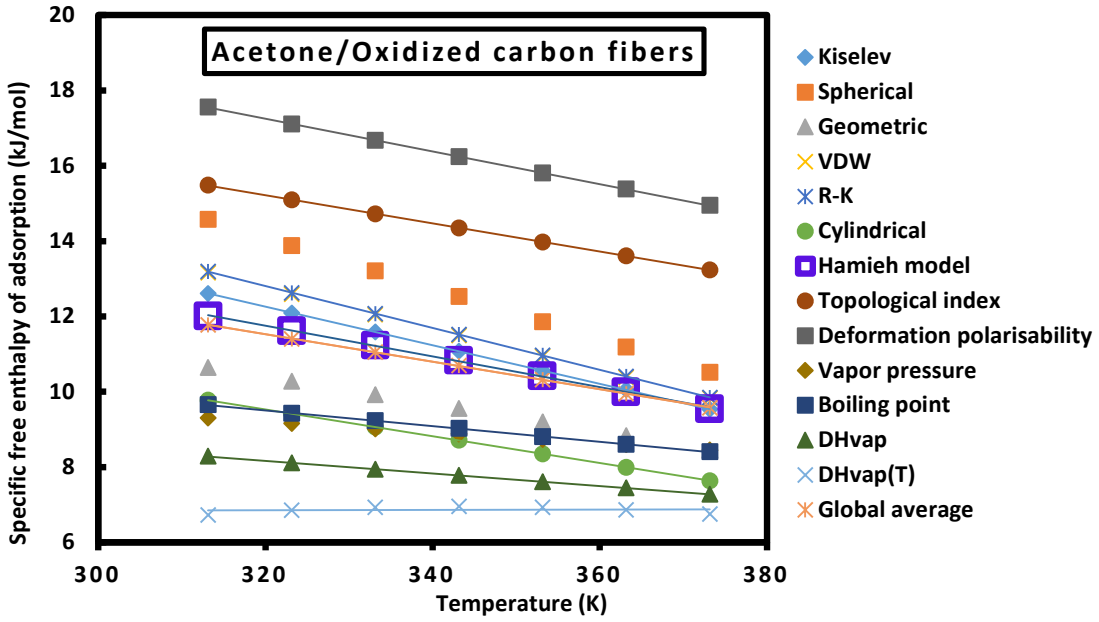

CH2Cl2/Oxidized carbon fibers
Specific free enthalpy of adsorption (kJ/mol)
Temperature (K)
0
2
4
6
8
10
12
14
16
300
320
340
360
380
Kiselev
Spherical
Geometric
VDW
R-K
Cylindrical
Hamieh model
Topological index
Deformation polarisability
Vapor pressure
Boiling point
DHvap
DHvap(T)
Global average


CHCl3/Oxidized carbon fibers
Specific free enthalpy of adsorption (kJ/mol)
Temperature (K)
0
2
4
6
8
10
12
14
16
18
20
300
320
340
360
380
Kiselev
Spherical
Geometric
VDW
R-K
Cylindrical
Hamieh model
Topological index
Deformation polarisability
Vapor pressure
Boiling point
DHvap
DHvap(T)
Global average


Benzene/Oxidized carbon fibers
Specific free enthalpy of adsorption (kJ/mol)
Temperature (K)
0
1
2
3
4
5
6
7
8
9
10
300
320
340
360
380
Kiselev
Spherical
Geometric
VDW
R-K
Cylindrical
Hamieh model
Topological index
Deformation polarisability
Vapor pressure
Boiling point
DHvap
DHvap(T)
Global average


THF/Oxidized carbon fibers
Specific free enthalpy of adsorption (kJ/mol)
Temperature (K)
Kiselev
Spherical
Geometric
VDW
R-K
Cylindrical
Hamieh model
Topological index
Deformation polarisability
Vapor pressure
Boiling point
DHvap
DHvap(T)
Global average


Ethyl acetate/Oxidized carbon fibers
Specific free enthalpy of adsorption (kJ/mol)
Temperature (K)
Kiselev
Spherical
Geometric
VDW
R-K
Cylindrical
Hamieh model
Topological index
Deformation polarisability
Vapor pressure
Boiling point
DHvap
DHvap(T)
Global average

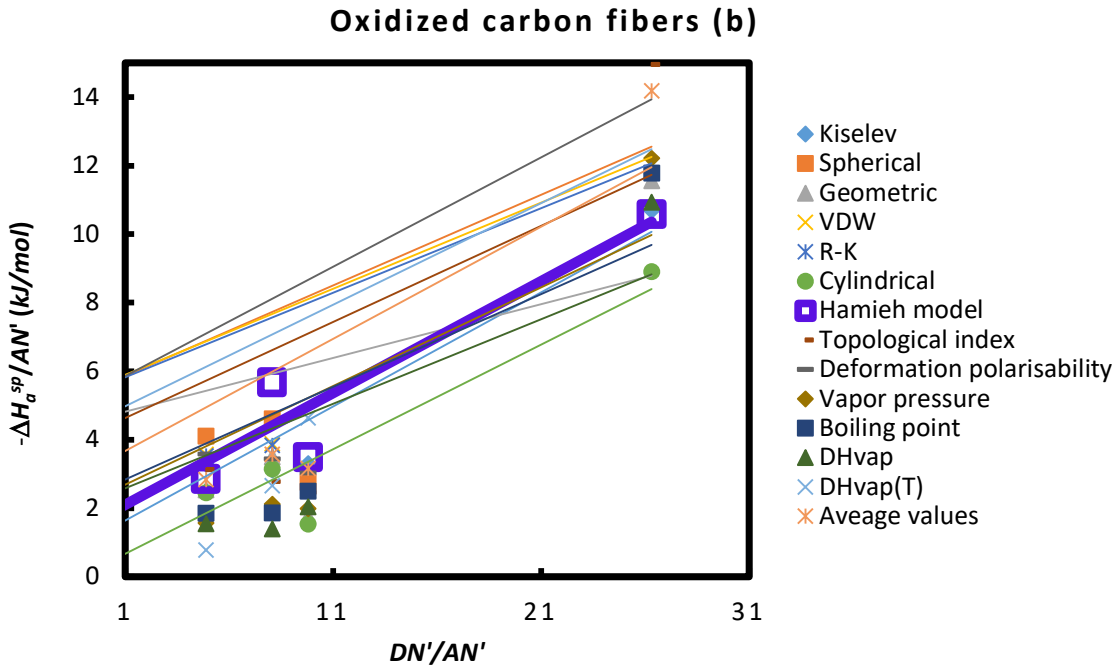


Figures S4. Variations of ΔG_a^{sp} of the various solvents adsorbed on oxidized carbon fibers as a function of the temperature for the different models and chromatographic methods.

Table S8. Variations of $(-\Delta S_a^{sp} in\ J\ K^{-1}mol^{-1})$ as a function of the used models or methods of polar molecules adsorbed on carbon fibers (a) and (b).

Untreated carbon fibers (a)								
Probes	**CCl4**	**CH2Cl2**	**CHCl3**	**Benzene**	**Ether**	**THF**	**EA**	**Acetone**
Kiselev	0.8	2.0	18.5	0.8	28.3	27.2	22.5	35.3
Spherical	7.8	11.4	-10.9	22.1	20.3	43.6	37.4	49.7
Geometric	11.7	32.6	78.6	9.7	17.2	29.1	21.1	22.4
VDW	3.8	10.3	15.5	23.2	21.1	45.1	30.5	41.7
R-K	3.7	9.8	14.3	21.4	19.6	41.6	28.1	38.4
Cylindrical	0.8	38.8	71.0	-6.6	14.2	23.3	22.7	24.9
Hamieh model	0.8	2.0	18.5	0.6	20.0	14.1	37.2	24.6
Topological index	-2.7	31.5	111.8	3.9	25.2	31.5	5.2	15.7
Deformation polarizability	0.0	14.2	104.5	7.7	27.4	36.0	8.0	17.8
Vapor pressure	13.5	15.2	96.1	2.6	19.1	30.1	-3.7	0.0
Boiling point	-14.7	0.0	98.4	3.4	25.1	26.5	1.2	6.5
ΔHvap	-14.4	15.9	98.8	2.9	23.4	25.2	-0.9	4.4
ΔHvap(T)	11.3	31.2	13.6	13.5	66.4	57.1	10.8	-14.6
Average values	1.7	16.5	56.1	8.1	25.2	33.1	16.9	20.5
Oxidized carbon fibers (b)								
Probes	**CCl4**	**CH2Cl2**	**CHCl3**	**Benzene**	**Ether**	**THF**	**EA**	**Acetone**

Kiselev	7.4	0	90.2	2.5	24	35.7	27.2	51.1
Spherical	15.1	13.6	-7.7	29.1	16.6	55.8	44.6	67.6
Geometric	24.6	33	5.1	15.1	9.3	38.5	28.3	36.5
VDW	12.1	11.4	-59.8	32	16.4	59.1	37.8	60.6
R-K	11.3	11	-53.8	29.4	15.4	54.4	34.8	55.7
Cylindrical	8.8	41.1	-7.3	-7.1	6.2	30.9	28.4	38.9
Hamieh model	8.2	5	28.7	7	30.2	24.4	50.2	40.8
Topological index	14.9	37.2	39.2	10.9	17.8	46.5	14.6	37.5
Deformation polarizability	18.9	5.2	25.6	17.9	22.1	54.9	19.9	43.5
Vapor pressure	-6.1	8.2	16.6	9.1	11.8	40.5	5.6	14.1
Boiling point	-7.3	16.8	14.4	9.8	18.2	37.4	7.2	20.8
ΔHvap	-6.6	8.5	15.2	9.1	14.7	34.9	3.5	16.7
ΔHvap(T)	17.9	25.2	49.9	22.5	56	64.6	18.9	0.0
Average values	9.2	16.6	12.0	14.4	19.9	44.4	24.7	37.2



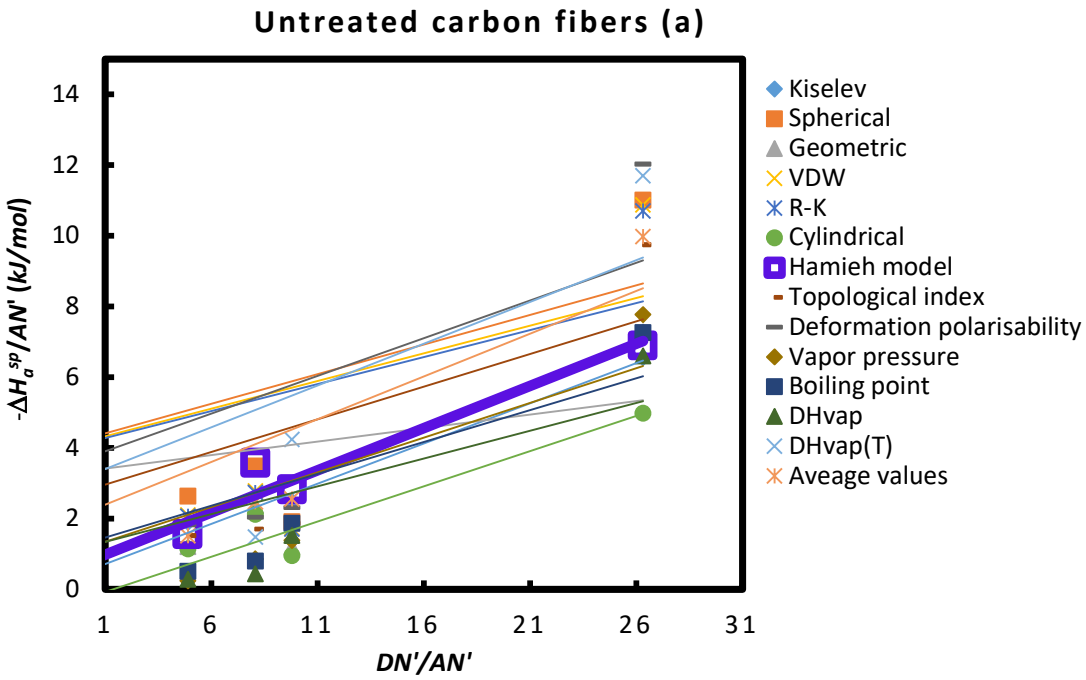
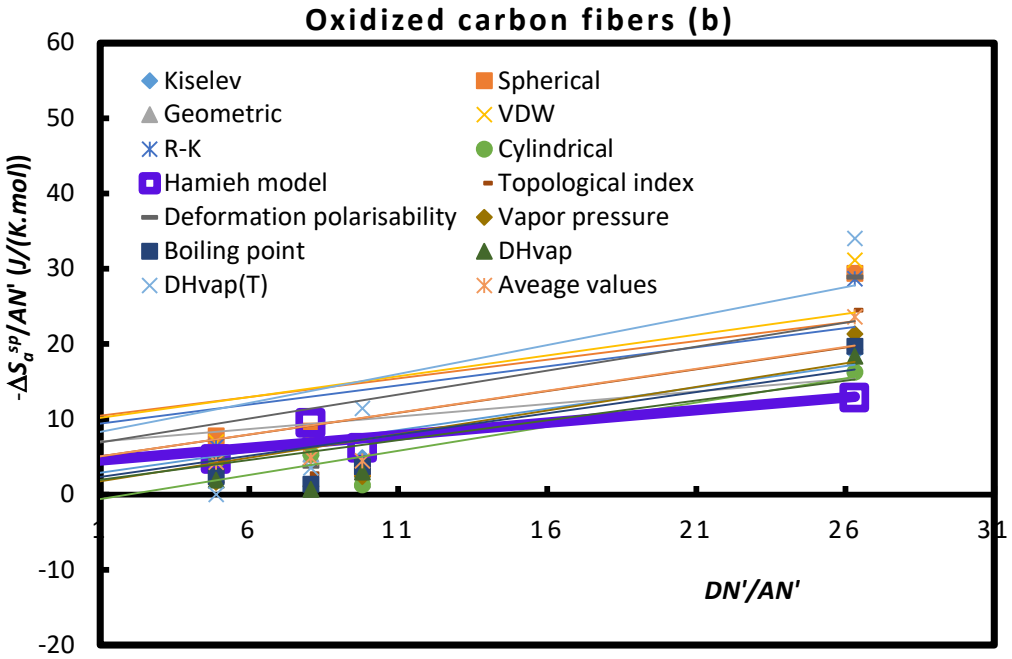


Figure S5. Variations of $\left(\frac{-\Delta H_a^{sp}}{AN'}\right)$ as a function of $\left(\frac{DN'}{AN'}\right)$ for different molecular models and IGC methods for the carbon fibers (a) and (b).



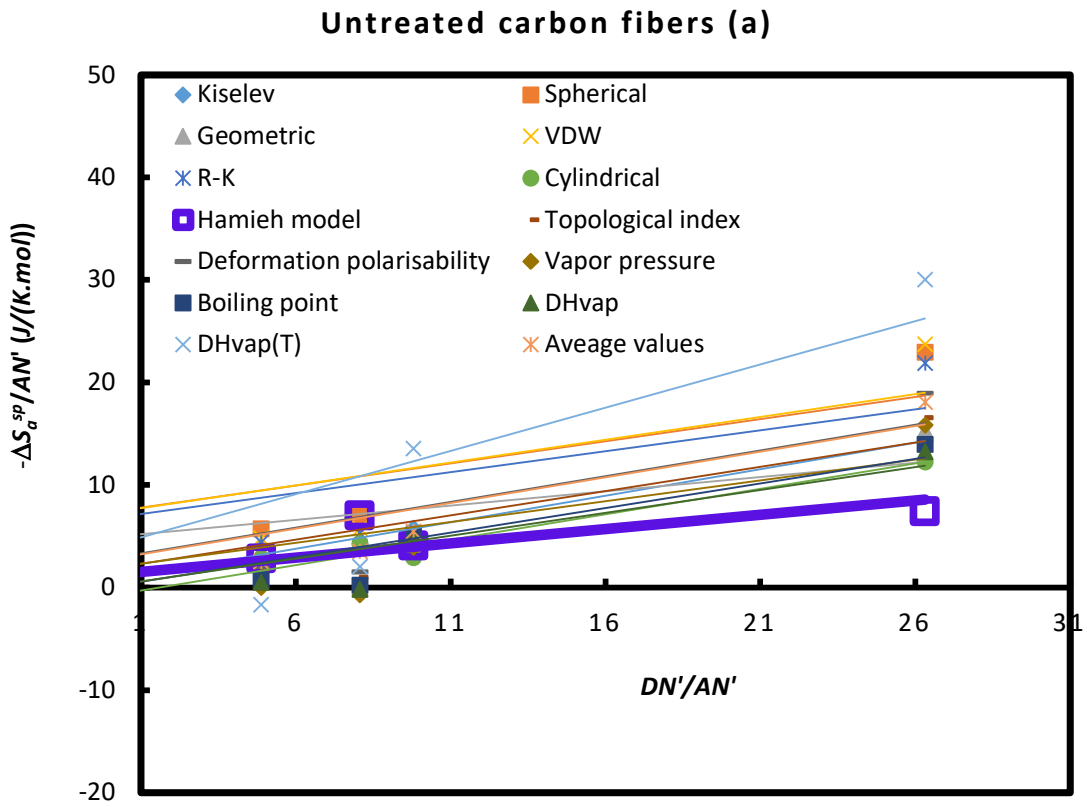


Figure S6. Variations of $\left(\frac{-\Delta S_a^{sp}}{AN'}\right)$ as a function of $\left(\frac{DN'}{AN'}\right)$ by using the various molecular models and IGC methods for the carbon fibers (a) and (b).