

Appendix E

Tabulated results from Monte-Carlo simulations of several *n*-alkane and ester penetrants.

HEXANE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
7.425	2.207	15.30	1.682
7.616	2.179	14.92	1.748
7.616	2.179	14.92	1.748
7.255	2.233	15.66	1.625
6.065	2.442	18.73	1.242
6.342	2.388	17.91	1.328
7.297	2.226	15.57	1.639
7.608	2.180	14.93	1.745
6.106	2.434	18.60	1.255
6.301	2.396	18.03	1.315
6.511	2.357	17.45	1.381
6.099	2.435	18.63	1.252
6.521	2.355	17.42	1.385
5.666	2.526	20.05	1.121
5.666	2.526	20.05	1.121
6.459	2.366	17.59	1.365
6.459	2.366	17.59	1.365
5.410	2.585	21.00	1.046

NONANE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
12.013	2.10672	13.94323	2.851114
11.255	2.176506	14.88227	2.585566
10.727	2.229428	15.6148	2.405774
10.89	2.212681	15.38108	2.460816
10.888	2.212884	15.38391	2.460138
11.178	2.18399	14.98479	2.559078
9.202	2.407086	18.20256	1.91144
9.824	2.329638	17.05008	2.108482
9.075	2.42387	18.4573	1.872006
9.844	2.32727	17.01544	2.114924
10.661	2.236319	15.71147	2.383605
10.391	2.265187	16.11972	2.29363
10.183	2.288204	16.44898	2.225107
10.386	2.265732	16.12748	2.291975
10.569	2.246031	15.84824	2.352817
9.893	2.3215	16.93116	2.130735
9.064	2.42534	18.4797	1.868604
8.93	2.44347	18.757	1.82732
8.624	2.486442	19.42254	1.734205
10.507	2.252648	15.94175	2.332144

DECANE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
13.293	2.110426	13.99233	3.149364
12.575	2.16984	14.79125	2.897679
12.578	2.169581	14.78772	2.898716
11.156	2.303708	16.67264	2.421314
10.492	2.375487	17.72779	2.20839
12.399	2.185186	15.00121	2.837058
11.662	2.253176	15.94924	2.587902
9.046	2.558312	20.56157	1.767963
10.325	2.39462	18.01453	2.155874
11.009	2.319038	16.89527	2.373614
10.959	2.324322	16.97235	2.357462
9.929	2.441906	18.733	2.033043
10.624	2.360683	17.50753	2.250196
11.999	2.22131	15.50129	2.700884
10.903	2.330283	17.05952	2.339415
11.821	2.237972	15.73471	2.641007
12.183	2.204472	15.26718	2.763247
12.005	2.220755	15.49354	2.70291
11.255	2.293554	16.52599	2.453616
9.84	2.452924	18.90244	2.005769

TRIDECANE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
17.108	2.110952	13.9993	4.0522
16.301	2.162574	14.69235	3.768889
15.657	2.206601	15.29667	3.547765
15.765	2.199029	15.19188	3.584536
12.263	2.493329	19.53029	2.459162
14.539	2.28987	16.47293	3.174635
15.085	2.248047	15.8767	3.355135
15.064	2.249613	15.89883	3.348131
15.234	2.237026	15.72141	3.404967
15.274	2.234095	15.68024	3.418387
14.519	2.291446	16.49563	3.168087
11.864	2.534909	20.18712	2.340123
10.975	2.635577	21.82232	2.082087
10.966	2.636659	21.84023	2.079526
14.367	2.303536	16.67015	3.118467
12.25	2.494652	19.55102	2.455252
15.1	2.24693	15.86093	3.36014
9.457	2.839235	25.32516	1.665414
14.974	2.256364	15.99439	3.318171
7.82	3.1223	30.6266	1.252282

PENTADECANE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
19.655	2.093015	13.7624	4.695379
17.578	2.213218	15.38855	3.971141
17.543	2.215424	15.41926	3.959286
17.474	2.219794	15.48014	3.93595
16.335	2.295881	16.55953	3.557458
8.37	3.207349	32.3178	1.304816
16.934	2.254909	15.97378	3.754918
15.663	2.344614	17.27	3.340208
16.601	2.277413	16.2942	3.644706
14.452	2.440871	18.71713	2.960418
16.306	2.297921	16.58899	3.547989
17.287	2.231768	15.6476	3.872938
16.928	2.255309	15.97944	3.752923
9.519	3.007553	28.41685	1.582516
10.698	2.836989	25.2851	1.88545
16.479	2.285828	16.41483	3.604603
12.063	2.67166	22.42394	2.257585
9.543	3.003768	28.34538	1.588505
14.627	2.426226	18.4932	3.014352
14.664	2.423163	18.44654	3.025797

HEXADECANE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
20.934	2.103515	13.90083	4.975957
17.97	2.270376	16.19366	3.957495
10.308	2.997675	28.2305	1.719333
16.353	2.379978	17.7949	3.435535
9.152	3.181367	31.79633	1.438376
14.462	2.530798	20.1217	2.857201
10.244	3.007024	28.40687	1.703345
11.038	2.896854	26.36347	1.90517
17.332	2.311785	16.78975	3.748619
14.333	2.542162	20.3028	2.819057
11.82	2.799387	24.61929	2.111176
11.03	2.897904	26.38259	1.9031
10.597	2.956516	27.4606	1.792143
11.385	2.852366	25.55995	1.995712
17.207	2.320167	16.91172	3.708139
17.207	2.320167	16.91172	3.708139
13.745	2.595968	21.17134	2.647374
10.032	3.038631	29.00718	1.650743
14.476	2.529574	20.10224	2.861351
18.266	2.251905	15.93124	4.055678

HEPTADECANE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
22.204	2.10299	13.89389	5.27915
19.291	2.256189	15.99191	4.27513
17.522	2.367342	17.60644	3.700775
10.57	3.048003	29.18638	1.733922
16.02	2.475834	19.25718	3.235273
13.037	2.744505	23.66342	2.37511
18.865	2.281521	16.35303	4.134304
10.485	3.060332	29.42299	1.713049
17.746	2.352354	17.3842	3.771967
16.078	2.471365	19.18771	3.252859
11.473	2.925596	26.88922	1.960797
10.153	3.109966	30.38511	1.632333
9.506	3.21406	32.45319	1.478815
10.046	3.126484	30.70874	1.606597
19.206	2.261176	16.06269	4.246905
11.012	2.986206	28.01489	1.843811
11.524	2.919115	26.77022	1.973886
10.971	2.99178	28.11959	1.833524
9.798	3.165805	31.48602	1.547474
18.488	2.304665	16.6865	4.010995

ETHYL PROPIONATE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
7	2.22633	15.57143	1.572094
7.171	2.199625	15.20011	1.630051
7.448	2.158334	14.6348	1.725405
6.766	2.264501	16.10996	1.493927
7.363	2.170756	14.80375	1.695953
7.544	2.144557	14.44857	1.758871
7.016	2.22379	15.53592	1.577487

ETHYL HEPTANOATE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
13.004	2.093212	13.765	3.106231
11.659	2.210656	15.35295	2.637
12.437	2.140395	14.39254	2.905305
11.194	2.256104	15.99071	2.480825
8.407	2.603342	21.29178	1.614655
9.002	2.515836	19.88447	1.789068
8.967	2.520741	19.96208	1.778644
8.587	2.575912	20.84546	1.666788
12.298	2.152457	14.55521	2.856735
7.314	2.791093	24.47361	1.310239
11.245	2.250982	15.91819	2.497799
7.417	2.771645	24.13375	1.338014
11.733	2.203673	15.25612	2.662146
6.699	2.916398	26.72041	1.148506
11.514	2.224532	15.54629	2.58796
11.767	2.200487	15.21203	2.673726
9.165	2.493363	19.53082	1.837879
7.589	2.740056	23.58677	1.384826
7.825	2.69842	22.8754	1.449922
7.162	2.820555	24.99302	1.269608

ETHYL NONOATE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
15.553	2.090341	13.72726	3.720207
7.661	2.978389	27.86842	1.286098
13.595	2.235808	15.7043	3.040287
11.481	2.432956	18.59594	2.359475
8.707	2.793765	24.5205	1.558291
14.846	2.139535	14.38098	3.469445
7.722	2.966602	27.64828	1.301489
10.061	2.598984	21.22055	1.935564
13.218	2.267469	16.15222	2.914704
8.117	2.89352	26.30282	1.402617
14.204	2.187353	15.03098	3.246847
9.511	2.673075	22.44769	1.779037
8.297	2.861961	25.73219	1.449531
11.023	2.482986	19.36859	2.219706
9.519	2.671951	22.42883	1.781283
13.926	2.209078	15.33104	3.151994
12.816	2.302756	16.65886	2.782752
12.791	2.305005	16.69142	2.774614
13.245	2.265156	16.11929	2.923639
13.127	2.275315	16.26419	2.884656

ETHYL MYRISTATE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
21.927	2.085134	13.65896	5.257934
9.451	3.176031	31.68977	1.487863
20.201	2.172387	14.826	4.649494
20.138	2.175783	14.87238	4.62776
16.983	2.36928	17.63528	3.584
18.132	2.292983	16.51776	3.953802
10.853	2.963799	27.59606	1.830927
18.756	2.254517	15.96822	4.159649
9.869	3.108043	30.34755	1.587655
9.356	3.192115	32.01154	1.465486
15.213	2.503319	19.68711	3.038566
8.739	3.30288	34.27166	1.322936
17.823	2.312774	16.80413	3.853165
10.137	3.066683	29.54523	1.652763
17.483	2.335155	17.13093	3.743435
16.586	2.397468	18.0574	3.459066
14.612	2.554282	20.49685	2.860295
11.392	2.892835	26.29038	1.969003
17.41	2.340045	17.20276	3.720013
15.598	2.472232	19.20118	3.154639

ISOPROPYL MYRISTATE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
14.238	2.666333	22.3346	2.66996
13.622	2.725953	23.34459	2.498576
21.904	2.149696	14.5179	5.094673
15.661	2.542313	20.30522	3.080069
11.163	3.011261	28.48697	1.853543
8.561	3.43856	37.14519	1.244853
20.579	2.217822	15.45265	4.639462
20.215	2.2377	15.73089	4.516914
19.04	2.305713	16.70168	4.128874
10.541	3.098831	30.16792	1.700803
11.846	2.923162	26.8445	2.02623
11.288	2.994541	28.17151	1.884763
11.713	2.939712	27.14932	1.992202
11.207	3.005344	28.37512	1.864512
11.87	2.920206	26.79023	2.032391
18.069	2.366856	17.5992	3.81709
17.71	2.390724	17.95596	3.703898
9.701	3.230208	32.78013	1.501606
17.71	2.390724	17.95596	3.703898
18.069	2.366856	17.5992	3.81709

ISODECYL PELARGONATE

Atom-atom dist. (Å)	Radius (Å)	X-sect. Area (Å ²)	Aspect Ratio (L/2R)
9.997	3.182028	31.80954	1.570854
11.029	3.029498	28.83308	1.820268
9.736	3.224397	32.66228	1.50974
8.824	3.386929	36.03808	1.302655
10.07	3.170473	31.57895	1.588091
8.776	3.396178	36.23519	1.29204
9.885	3.200004	32.16995	1.54453
8.776	3.396178	36.23519	1.29204
10.147	3.158421	31.33931	1.606341
9.259	3.30641	34.34496	1.400159
8.75	3.40122	36.34286	1.286303
8.955	3.362064	35.51089	1.331771
8.395	3.47239	37.87969	1.208822
11.309	2.99176	28.1192	1.890025
10.319	3.131987	30.81694	1.647357
10.566	3.095163	30.09654	1.706857
8.006	3.555748	39.72021	1.125783
9.602	3.246818	33.1181	1.478678
9.754	3.221421	32.60201	1.513928
21.834	3.465174	37.72242	1.216389