**Supplementary Material**

*Correlation of the Simulation Data*

The simulation data for the thermal conductivity of the saturated liquid and the surface tension are correlated with the Matlab Curve Fitting Tool. The method used is Nonlinear Least Squares with a Trust-Region algorithm and the functional form chosen is the same as for the experimental correlations from DIPPR [1]. The data for the liquid thermal conductivity is gathered from Fernández et al. [2] and depends on the reduced liquid density $\rho'^*$. To get a data set which is dependent on the reduced temperature $T^*$ an additional correlation $T^*(\rho'^*)$ is needed. The data set is taken from Lotfi et al. [3] and the following function is used:

$$T^*(\rho'^*) = A(\rho'^*)^2 + B\rho'^* + C \tag{1}$$

The coefficients are $A = -2.513$, $B = 1.734$ and $C = 1.02$ and the root-mean-square-error (RMSE) for the fit is 0.2%. The transferred data set for the liquid thermal conductivity in reduced units is fitted by:

$$\lambda'^*(T^*) = A(T^*)^2 + BT^* + C \tag{2}$$

The coefficients are $A = -7.925$, $B = 6.995$ and $C = 5.764$ with a RMSE of 29%. In Figure S.1 the data set (+) and the correlation (-) of the liquid thermal conductivity are plotted. In Figure S.2 the corresponding deviation plot can be found.

The data set for the surface tension in reduced units is from Grosfils et al. [4] and fitted by:

$$\gamma^*(T^*) = A\left(1 - \frac{T^*}{B}\right)^C \tag{3}$$

The coefficients are $A = 2.982$, $B = 1.3126$ and $C = 1.338$ with a RMSE of 0.4%. In Figure S.3 the data set (+) and the correlation (-) of the surface tension are plotted. In Figure S.4 the corresponding deviation plot can be found.

*List of Tables*

**Table S.1**

| ID | $\frac{\epsilon}{k}$ / K | $\sigma$ / Å | $\delta\rho'/\%$ | $\delta p^S/\%$ | $\delta\Delta h_V/\%$ | $\delta\eta'/\%$ | $\delta\lambda'/\%$ | $\delta\gamma'/\%$ |
|---|---|---|---|---|---|---|---|---|
| 1 | 115.40 | 3.44 | 4.554 | 4.274 | 0.900 | 8.495 | 7.763 | 0.658 |
| 2 | 115.60 | 3.42 | 2.705 | 4.916 | 0.504 | 7.844 | 6.574 | 2.480 |
| 3 | 115.60 | 3.43 | 3.552 | 4.086 | 0.504 | 8.060 | 6.973 | 1.898 |
| 4 | 115.60 | 3.44 | 4.390 | 3.307 | 0.504 | 8.306 | 7.388 | 1.332 |
| 5 | 115.80 | 3.41 | 1.686 | 4.741 | 0.441 | 7.660 | 5.850 | 4.455 |
| 6 | 115.80 | 3.42 | 2.540 | 3.904 | 0.441 | 7.794 | 6.215 | 3.862 |
| 7 | 115.80 | 3.43 | 3.387 | 3.119 | 0.441 | 7.965 | 6.605 | 3.281 |
| 8 | 115.80 | 3.44 | 4.225 | 2.426 | 0.441 | 8.170 | 7.013 | 2.715 |
| 9 | 116.00 | 3.40 | 0.706 | 4.573 | 0.809 | 7.684 | 5.195 | 6.535 |
| 10 | 116.00 | 3.41 | 1.530 | 3.729 | 0.809 | 7.724 | 5.510 | 5.935 |
| 11 | 116.00 | 3.42 | 2.378 | 2.938 | 0.809 | 7.807 | 5.860 | 5.345 |
| 12 | 116.00 | 3.43 | 3.223 | 2.242 | 0.809 | 7.931 | 6.238 | 4.766 |
| 13 | 116.00 | 3.44 | 4.061 | 1.741 | 0.809 | 8.091 | 6.638 | 4.202 |
| 14 | 116.00 | 3.45 | 4.891 | 1.610 | 0.809 | 8.285 | 7.055 | 3.657 |
| 15 | 116.20 | 3.39 | 0.610 | 4.412 | 1.288 | 7.922 | 4.647 | 8.702 |
| 16 | 116.20 | 3.40 | 0.611 | 3.562 | 1.288 | 7.866 | 4.887 | 8.091 |
| 17 | 116.20 | 3.41 | 1.381 | 2.764 | 1.288 | 7.855 | 5.177 | 7.490 |
| 18 | 116.20 | 3.42 | 2.219 | 2.064 | 1.288 | 7.886 | 5.509 | 6.900 |
| 19 | 116.20 | 3.43 | 3.061 | 1.580 | 1.288 | 7.960 | 5.873 | 6.321 |
| 20 | 116.20 | 3.44 | 3.898 | 1.513 | 1.288 | 8.072 | 6.263 | 5.756 |
| 21 | 116.40 | 3.38 | 1.602 | 4.260 | 1.798 | 8.368 | 4.256 | 10.951 |
| 22 | 116.40 | 3.39 | 0.804 | 3.403 | 1.798 | 8.219 | 4.390 | 10.329 |
| 23 | 116.40 | 3.40 | 0.572 | 2.596 | 1.798 | 8.113 | 4.594 | 9.716 |
| 24 | 116.40 | 3.41 | 1.245 | 1.892 | 1.798 | 8.051 | 4.855 | 9.113 |
| 25 | 116.40 | 3.42 | 2.065 | 1.425 | 1.798 | 8.031 | 5.165 | 8.521 |
| 26 | 116.40 | 3.43 | 2.901 | 1.430 | 1.798 | 8.054 | 5.513 | 7.940 |
| 27 | 116.60 | 3.38 | 1.806 | 3.251 | 2.325 | 8.768 | 4.077 | 12.653 |
| 28 | 116.60 | 3.39 | 1.004 | 2.436 | 2.325 | 8.575 | 4.160 | 12.027 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 29 | 116.60 | 3.40 | 0.603 | 1.724 | 2.325 | 8.422 | 4.320 | 11.411 |
| 30 | 116.60 | 3.41 | 1.128 | 1.278 | 2.325 | 8.310 | 4.548 | 10.804 |
| 31 | 116.60 | 3.42 | 1.918 | 1.363 | 2.325 | 8.241 | 4.830 | 10.208 |
| 32 | 116.80 | 3.38 | 2.014 | 2.282 | 2.866 | 9.218 | 3.938 | 14.426 |
| 33 | 116.80 | 3.39 | 1.209 | 1.562 | 2.866 | 8.984 | 3.962 | 13.796 |
| 34 | 116.80 | 3.40 | 0.697 | 1.138 | 2.866 | 8.787 | 4.072 | 13.175 |
| 35 | 116.80 | 3.41 | 1.036 | 1.311 | 2.866 | 8.630 | 4.258 | 12.564 |
| 36 | 117.00 | 3.39 | 1.417 | 1.008 | 3.418 | 9.442 | 3.803 | 15.640 |
| 37 | 117.00 | 3.40 | 0.835 | 1.276 | 3.418 | 9.206 | 3.855 | 15.013 |
| 38 | 117.00 | 3.41 | 0.979 | 1.938 | 3.418 | 9.006 | 3.991 | 14.396 |
| 39 | 117.20 | 3.38 | 2.438 | 0.886 | 3.981 | 10.250 | 3.797 | 18.204 |
| 40 | 117.20 | 3.39 | 1.629 | 1.256 | 3.981 | 9.945 | 3.689 | 17.562 |
| 41 | 117.20 | 3.40 | 1.000 | 1.972 | 3.981 | 9.672 | 3.676 | 16.929 |
| 42 | 117.20 | 3.41 | 0.964 | 2.768 | 3.981 | 9.434 | 3.755 | 16.305 |
| 43 | 117.40 | 3.37 | 3.522 | 0.777 | 4.556 | 11.187 | 4.065 | 20.875 |
| 44 | 117.40 | 3.39 | 1.844 | 2.011 | 4.556 | 10.489 | 3.627 | 19.567 |
| 45 | 117.40 | 3.40 | 1.184 | 2.828 | 4.556 | 10.183 | 3.542 | 18.927 |
| 46 | 117.40 | 3.41 | 0.997 | 3.656 | 4.556 | 9.909 | 3.555 | 18.297 |
| 47 | 117.40 | 3.42 | 1.458 | 4.484 | 4.556 | 9.668 | 3.662 | 17.675 |

**Table S.2**

| ID | $\frac{\epsilon}{k}$ / K | $\sigma$ / Å | $\delta\rho'/\%$ | $\delta p^S/\%$ | $\delta\Delta h_V/\%$ | $\delta\eta'/\%$ | $\delta\lambda'/\%$ | $\delta\gamma'/\%$ |
|---|---|---|---|---|---|---|---|---|
| 1 | 147.25 | 3.77 | 3.885 | 4.793 | 1.407 | 19.280 | 4.839 | 5.963 |
| 2 | 147.25 | 3.78 | 4.646 | 4.102 | 1.407 | 18.658 | 5.293 | 6.374 |
| 3 | 147.50 | 3.76 | 2.997 | 4.466 | 1.118 | 20.549 | 4.111 | 4.853 |
| 4 | 147.50 | 3.77 | 3.766 | 3.782 | 1.118 | 19.918 | 4.552 | 5.239 |
| 5 | 147.50 | 3.78 | 4.528 | 3.170 | 1.118 | 19.293 | 5.002 | 5.642 |
| 6 | 147.75 | 3.74 | 1.315 | 4.878 | 0.883 | 22.480 | 3.037 | 3.529 |
| 7 | 147.75 | 3.75 | 2.100 | 4.147 | 0.883 | 21.835 | 3.422 | 3.820 |
| 8 | 147.75 | 3.76 | 2.877 | 3.469 | 0.883 | 21.195 | 3.835 | 4.153 |
| 9 | 147.75 | 3.77 | 3.647 | 2.875 | 0.883 | 20.560 | 4.268 | 4.519 |
| 10 | 147.75 | 3.78 | 4.410 | 2.417 | 0.883 | 19.931 | 4.713 | 4.908 |
| 11 | 148.00 | 3.73 | 0.427 | 4.563 | 0.757 | 23.791 | 2.500 | 2.836 |
| 12 | 148.00 | 3.74 | 1.197 | 3.835 | 0.757 | 23.137 | 2.806 | 2.974 |
| 13 | 148.00 | 3.75 | 1.980 | 3.165 | 0.757 | 22.488 | 3.167 | 3.195 |
| 14 | 148.00 | 3.76 | 2.758 | 2.592 | 0.757 | 21.844 | 3.566 | 3.479 |
| 15 | 148.00 | 3.77 | 3.528 | 2.181 | 0.757 | 21.206 | 3.988 | 3.811 |
| 16 | 148.00 | 3.78 | 4.291 | 2.024 | 0.757 | 20.573 | 4.427 | 4.178 |
| 17 | 148.25 | 3.72 | 0.590 | 4.256 | 0.797 | 25.119 | 2.171 | 2.664 |
| 18 | 148.25 | 3.73 | 0.343 | 3.530 | 0.797 | 24.455 | 2.333 | 2.551 |
| 19 | 148.25 | 3.74 | 1.082 | 2.869 | 0.797 | 23.797 | 2.594 | 2.549 |
| 20 | 148.25 | 3.75 | 1.861 | 2.321 | 0.797 | 23.144 | 2.925 | 2.656 |
| 21 | 148.25 | 3.76 | 2.638 | 1.970 | 0.797 | 22.497 | 3.304 | 2.857 |
| 22 | 148.25 | 3.77 | 3.409 | 1.915 | 0.797 | 21.855 | 3.713 | 3.132 |
| 23 | 148.25 | 3.78 | 4.172 | 2.170 | 0.797 | 21.218 | 4.143 | 3.462 |
| 24 | 148.25 | 3.79 | 4.928 | 2.639 | 0.797 | 20.587 | 4.587 | 3.831 |
| 25 | 148.50 | 3.72 | 0.724 | 3.232 | 0.988 | 25.791 | 2.113 | 2.787 |
| 26 | 148.50 | 3.73 | 0.297 | 2.582 | 0.988 | 25.123 | 2.202 | 2.513 |
| 27 | 148.50 | 3.74 | 0.970 | 2.066 | 0.988 | 24.461 | 2.407 | 2.337 |
| 28 | 148.50 | 3.75 | 1.744 | 1.788 | 0.988 | 23.804 | 2.700 | 2.279 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 29 | 148.50 | 3.76 | 2.519 | 1.849 | 0.988 | 23.153 | 3.052 | 2.343 |
| 30 | 148.50 | 3.77 | 3.290 | 2.212 | 0.988 | 22.508 | 3.445 | 2.518 |
| 31 | 148.50 | 3.78 | 4.054 | 2.752 | 0.988 | 21.868 | 3.864 | 2.781 |
| 32 | 148.50 | 3.79 | 4.810 | 3.381 | 0.988 | 21.233 | 4.300 | 3.108 |
| 33 | 148.75 | 3.72 | 0.859 | 2.305 | 1.264 | 26.466 | 2.105 | 3.141 |
| 34 | 148.75 | 3.73 | 0.307 | 1.828 | 1.264 | 25.795 | 2.113 | 2.744 |
| 35 | 148.75 | 3.74 | 0.863 | 1.643 | 1.264 | 25.129 | 2.251 | 2.410 |
| 36 | 148.75 | 3.75 | 1.628 | 1.829 | 1.264 | 24.469 | 2.495 | 2.164 |
| 37 | 148.75 | 3.76 | 2.401 | 2.288 | 1.264 | 23.814 | 2.815 | 2.036 |
| 38 | 148.75 | 3.77 | 3.171 | 2.887 | 1.264 | 23.165 | 3.186 | 2.043 |
| 39 | 148.75 | 3.78 | 3.935 | 3.549 | 1.264 | 22.521 | 3.591 | 2.182 |
| 40 | 148.75 | 3.79 | 4.691 | 4.242 | 1.264 | 21.883 | 4.018 | 2.427 |
| 41 | 149.00 | 3.73 | 0.371 | 1.541 | 1.584 | 26.470 | 2.074 | 3.197 |
| 42 | 149.00 | 3.75 | 1.513 | 2.394 | 1.584 | 25.137 | 2.318 | 2.365 |
| 43 | 149.00 | 3.76 | 2.283 | 3.038 | 1.584 | 24.478 | 2.595 | 2.047 |
| 44 | 149.00 | 3.77 | 3.052 | 3.728 | 1.584 | 23.826 | 2.939 | 1.837 |
| 45 | 149.00 | 3.78 | 3.816 | 4.437 | 1.584 | 23.178 | 3.325 | 1.768 |
| 46 | 149.25 | 3.71 | 1.921 | 1.424 | 1.928 | 28.513 | 2.511 | 4.847 |
| 47 | 149.25 | 3.72 | 1.132 | 1.486 | 1.928 | 27.828 | 2.243 | 4.318 |
| 48 | 149.25 | 3.74 | 0.678 | 2.523 | 1.928 | 26.476 | 2.063 | 3.302 |
| 49 | 149.25 | 3.77 | 2.934 | 4.635 | 1.928 | 24.490 | 2.706 | 2.000 |
| 50 | 149.50 | 3.70 | 2.875 | 1.271 | 2.287 | 29.898 | 3.094 | 6.152 |
| 51 | 149.50 | 3.74 | 0.610 | 3.376 | 2.287 | 27.156 | 2.044 | 3.974 |
| 52 | 149.75 | 3.69 | 3.845 | 1.164 | 2.656 | 31.301 | 3.804 | 7.535 |
| 53 | 150.00 | 3.68 | 4.829 | 1.110 | 3.033 | 32.721 | 4.588 | 8.974 |

**List of Figures**

pressure ($\circ$), enthalpy of vaporization ($*$), liquid viscosity ($\square$), liquid thermal conductivity ($\triangle$) and surface tension ($\triangledown$). Only models with relative mean deviations below 5% for the liquid density, vapor pressure and enthalpy of vaporization. For numerical data see Supplementary Material.

- Figure S.9: Pareto set in parameter space for six objective functions of methane: liquid density, vapor pressure, enthalpy of vaporization, liquid viscosity, liquid thermal conductivity and surface tension. Left side: Full investigated range. Right side: Zoom plus models found in literature: OPLS-UA [5] ($\circ$), Fischer et al. [6] ($\square$), Shukla [7] ($\triangle$), Vrabec and Fischer [8] ($\triangledown$), TraPPE [9] ($\Diamond$), Vrabec et al. [10] ($*$).

- Figure S.10: Pareto set in parameter space for three objective functions of methane: liquid density $\rho'$, vapor pressure $p^S$ and enthalpy of vaporization $\Delta h_V$. Red dashed lines: path of lowest descent for properties. Red markers: Global minima of properties.

- Figure S.11: Pareto set in parameter space for six objective functions of methane: liquid density $\rho'$, vapor pressure $p^S$, enthalpy of vaporization $\Delta h_V$, liquid viscosity $\eta'$, liquid thermal conductivity $\lambda'$ and surface tension $\gamma$. Red dashed lines: path of lowest descent for properties. Red markers: Global minima of properties.

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