Supplemental materials for "The shear viscosity of rigid water models"

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A. Autocorrelation functions

Figure 1 shows the normalized autocorrelation functions (ACF) of the non-diagonal components of the pressure tensor for rigid water models at ambient conditions (298 K, 1 bar). Notice that almost all the models give similar values at the minimum and the first maximum. However the differences are very significant for the ACF tail. The behavior of TIP3P is somewhat different, the first maximum is quite low and the ACF has almost no structure beyond that point.

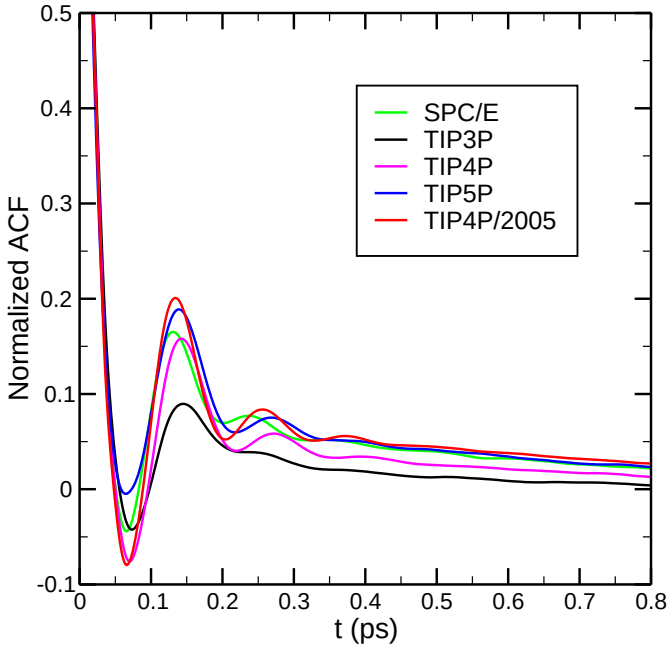

FIG. 1: Normalized autocorrelation functions at 298 K, 1 bar.

B. Limits of the integrals over the ACFs

Figure 2 shows the running values of the viscosities obtained by integration of the normalized ACFs displayed in Fig.1. Although the contribution of the low correlation times is not negligible, the main contribution comes from the tail of the ACF. Notice that all the systems exhibit a plateau after which the running viscosities are affected by the noise in the long tail. The upper limit in the integration to calculate the final value for the viscosity is taken at the beginning of the plateau. The effect of using a slightly different value (say, 1 Å beyond) is not significant; it amounts to a difference of about 0.003 mPa·s.

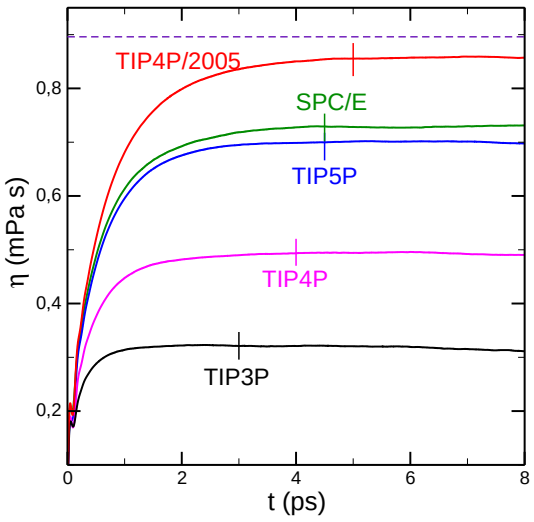

FIG. 2: Running values of the viscosity as a function of the correlation time for the systems shown in Fig. 1. The vertical lines indicate the upper limits used for the final results. The experimental result is displayed as a dashed line.

C. Effect of system size

Figure 3 shows the effect of the sample size in the calculated viscosities of TIP4P/2005 at 298 K, 1 bar. The departures are clearly within the statistical uncertainty.

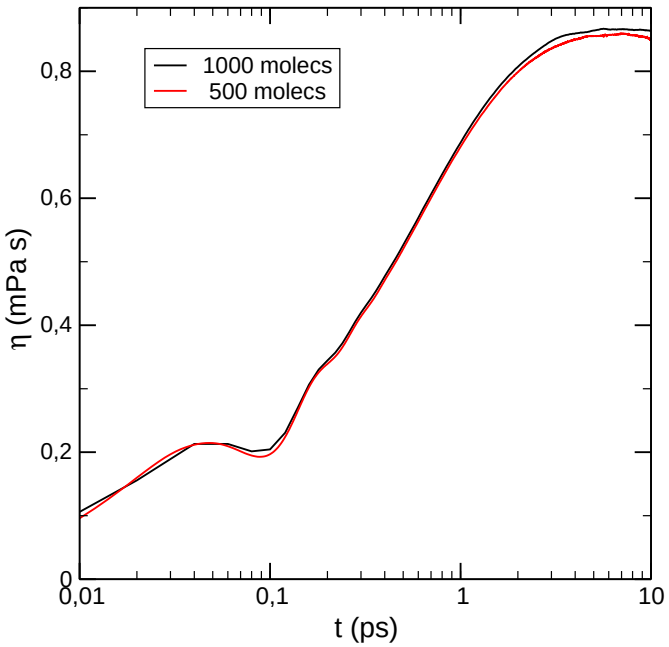

FIG. 3: Viscosity of TIP4P/2005 at ambient conditions for two different system samples: 500 and 1000 molecules.

D. Numerical values of the viscosity of rigid water models

TABLE I: Shear viscosity of rigid water models. The fifth column shows the upper limit in the integral over the autocorrelation functions and, the sixth, the simulation length.

Model	T/K	p/MPa	η/mPa·s	t_{max}(ps)	length(ns)
TIP3P	298	-1	0.321± 0.009	3.0	18
TIP4P	298	1	0.494± 0.013	4.0	30
TIP5P	298	0	0.699± 0.012	4.5	40
SPC/E	298	1	0.729± 0.013	4.5	20
SPC/E	298	100	0.718± 0.018	4.5	20
SPC/E	298	302	0.777± 0.022	4.5	20
SPC/E	298	495	0.844± 0.020	4.5	20
TIP4P/2005	373	-2	0.289± 0.008	4.0	20
TIP4P/2005	373	100	0.313± 0.008	4.0	20
TIP4P/2005	373	300	0.358± 0.009	4.0	20
TIP4P/2005	373	500	0.394± 0.008	4.0	20
TIP4P/2005	348	0	0.378± 0.009	4.5	20
TIP4P/2005	323	0	0.543± 0.010	4.5	20
TIP4P/2005	298	0	0.855± 0.013	5.0	40
TIP4P/2005	298	99	0.819± 0.019	5.0	30
TIP4P/2005	298	299	0.850± 0.019	5.0	30
TIP4P/2005	298	501	0.922± 0.022	5.0	30
TIP4P/2005	273	-1	1.66 ± 0.06	10.0	54
TIP4P/2005	273	100	1.34 ± 0.08	8.0	27
TIP4P/2005	273	201	1.42 ± 0.07	7.5	30
TIP4P/2005	273	298	1.45 ± 0.08	7.5	23
TIP4P/2005	273	501	1.54 ± 0.06	8.0	38