Simulation Foundry: scalable and FAIR molecular modelling

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1 Results

This report was generated using the workflow developed by G. Gygli in 2018-2019. It summarises the results of your simulations and allows you to easily get an overview of your data.
2 energy

This is a mixture of H2O and MEOH

Figure 1: Simple overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of simulation ensemble of a mixture of H2O and MEOH.
(e) Density, in g/cm$^3$

(f) Enthalpy, in kJ/mol

(g) Volume, in m$^3$

Figure 1: ... continued
Figure 2: Complex overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of simulation ensemble of a mixture of H2O and MEOH.
Figure 2: ... continued
Figure 3: Simple overview of experimentally measured density data (source1, source2).

Figure 4: Complex overview of experimentally measured density data (source1, source2).
3 Comparison experimental to simulation data (gmx energy keywords)

This is a comparison of experimental and simulation data of H2O and MEOH mixtures.

Figure 5: Comparing experimental and simulation data for properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of simulationensemble of a mixture of H2O and MEOH. Experimental data is shown in red. Temperature is in K and mole fraction of water in mol/mol.
The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

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Figure 5: ... continued
4 msd

This is a mixture of H2O and MEOH.

Figure 6: Simple overview of msd for selected groups (MEOH Water System) of simulation ensemble of a mixture of H2O and MEOH.
Figure 7: Complex overview of msd for selected groups (MEOH Water System) of simulation ensemble of a mixture of H2O and MEOH.
5 Comparison experimental to simulation data (Diffusion)

This is a comparison of experimental and simulation data of H2O and MEOH mixtures.

Figure 8: Comparing experimental and simulation data for Diffusion of simulation ensemble of a mixture of H2O and MEOH. Experimental data is shown in red. Experimental data is shown in red. Temperature is in K and mole fraction of water in mol/mol-
6 hbonds

This is a mixture of H2O and MEOH

Figure 9: Simple overview of hbonds of simulation ensemble of a mixture of H2O and MEOH
Figure 10: Complex overview of hbonds of simulation ensemble of a mixture of H2O and MEOH
6.1 Methods

Molecular dynamics simulations were performed with the GROningen MACHine for Chemical Simulation (GROMACS) package (GROMACS 5.1.4-gnu-4.9/2016.5, GROMACS1, GROMACS2, GROMACS3, GROMACS4, GROMACS5, GROMACS6, GROMACS7), on the high performance infrastructure of the hopen. A bash (version 4.4.19) script was used to simultaneously launch replicates of each of 1 solvent mixtures of molecules at different temperatures (20, degrees celsius), thus 33 simulations were performed in total. The oplsaa and spce water model were used (oplsaa, spce). Non-standard molecules were parametrized using the LigParGen webserver with the 1.14*CM1A charge model (LigParGen1, LigParGen2, LigParGen3).

A Simulation Foundry (DOI of our PUBLICATION) was used to automatically perform the ensemble of simulations (simulation foundry). The simulation box was 8 by 8 by 8 nm large, and was neutral due to the partial charges of the molecules in the system being zero. by adding 0 None ions.

Minimisation was performed for 50000 steps using steep (a steepest descent algorithm implemented in GROMACS). Equilibration was performed for 10 ns using the md integrator (a leap-frog algorithm implemented in GROMACS), the V-rescale thermostat (V-rescale) with isotropic coupling (tauT=0.1) and the barostat (), and electrostatic interactions were calculated with the particel-mesh Ewald summation (PME1, PME2). While equilibration was performed under NPT conditions, production was performed under NPT conditions by adding a Berendsen pressure coupling (Berendsen, tauP=0.6) for 100 ns. Check the mdp files of the Simulation Foundry for more parameters.