

Supplementary Material

In order to verify the correct working of the the thermodynamic control and stability of the simulations, the temperature and pressure fluctuations were monitored for all molecules in their respective environments under NVT, NPT and MD simulations.

- For the NVT and MD graphs of temperature, the values always stabilised at around 298K as shown by the horizontal, dashed, blue line.
- For the NPT and MD graphs of pressure, the values always stabilised at around 1bar as shown by the horizontal, dashed, blue line.

NVT Temperature Equilibration

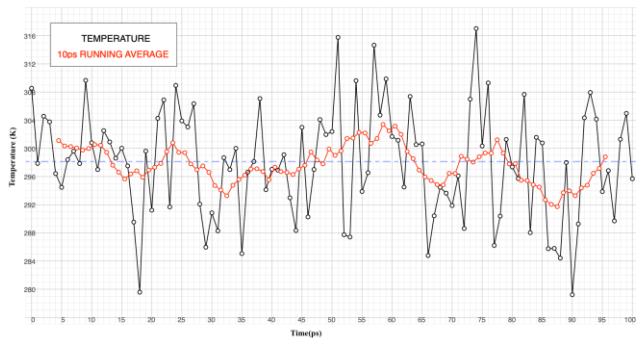


Figure A1 - CH₄ IN WATER

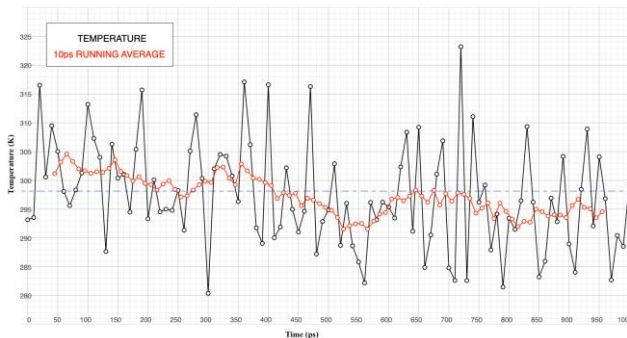


Figure A2 - CHF₃ IN WATER

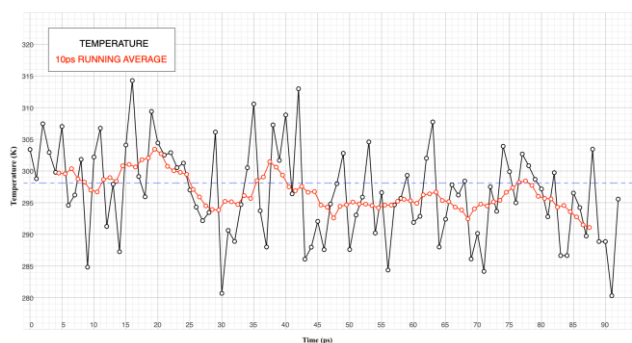


Figure A3 - CH₄ IN SALT WATER

NPT Pressure Equilibration

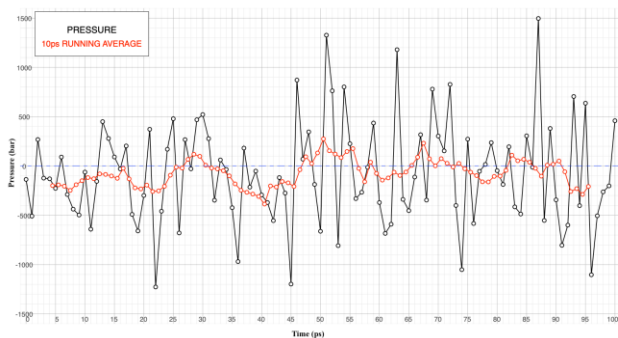


Figure B1 - CH₄ IN WATER

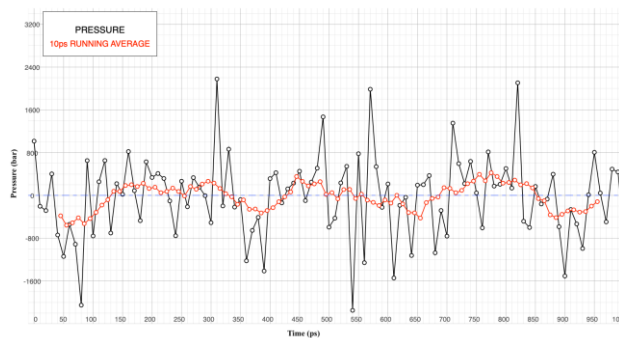


Figure B2 - CHF₃ IN WATER

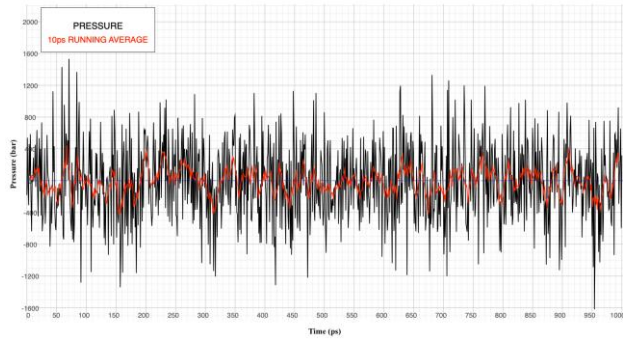


Figure B3 - CH₄ IN SALT WATER

MD Temperature Equilibration

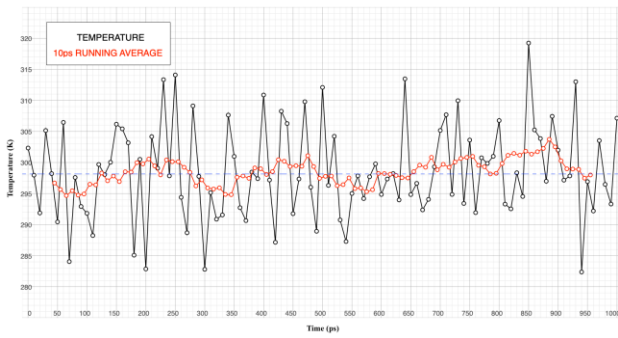


Figure C1 - CH₄ IN WATER

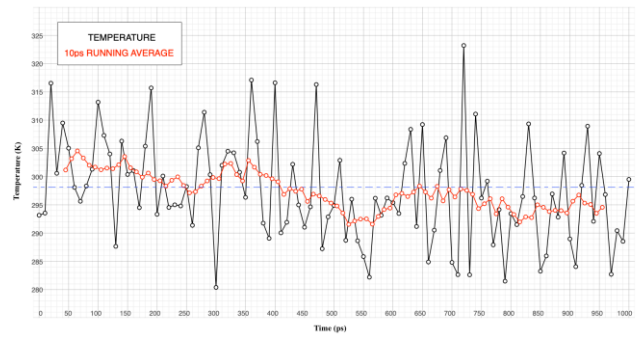


Figure C2 - CHF₃ IN WATER

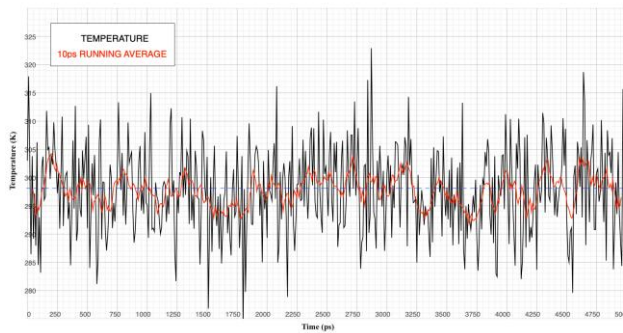
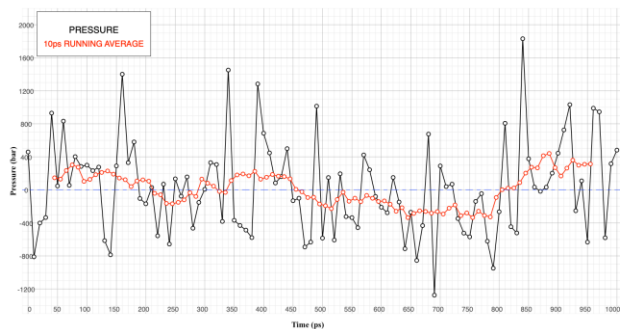


Figure C3 - CH₄ IN SALT WATER

MD Pressure Equilibration



D1 - CH₄ IN WATER

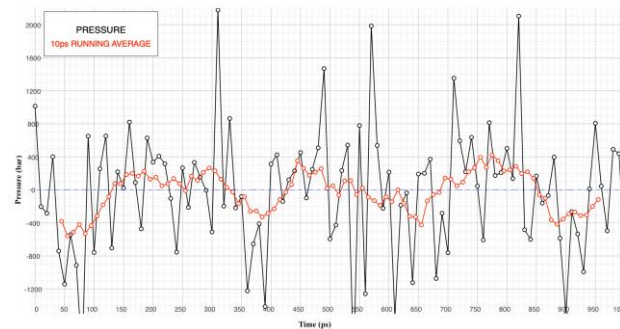


Figure D2 - CHF₃ IN WATER

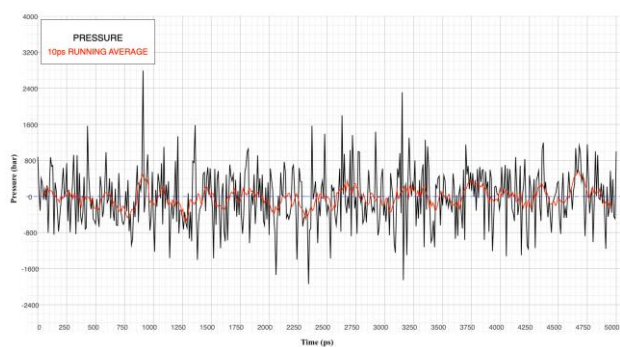


Figure D3 - CH₄ IN SALT WATER