

# HCl in Water Forces and Dynamics



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## Aim

The aim of this project was to analyze whether the computer model of hydrochloric acid in water was correct. Specifically we analyzed whether the model took dissociation of hydrochloric acid into account.

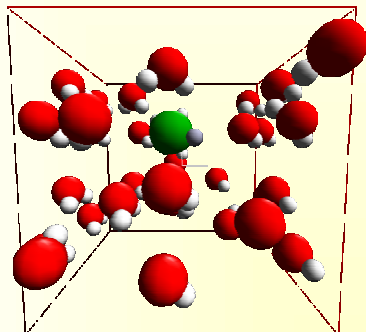


Figure 1. Image of the Computer Model

## Method

### The simulation model

In this simulation a cubic box ( $18.2 \times 18.2 \times 18.2 a_0$ ) was used. Periodicity of the system was implemented according to the minimum-system-image convention. The ratio of water to HCl molecules was 20 to 1. This meant the concentration in the simulation model was 2.8 M. The forces that influenced the water molecules were calculated according to the Ferguson model<sup>[1]</sup>.

In this model, the temperature was kept constant using a method called *weak coupling to an external bath*<sup>[2]</sup>. In this method, the velocity vectors of the particles in the simulation were rescaled to keep the temperature constant. In our simulation, the vectors were rescaled over a period of 8 ps. This meant that the dynamic properties of the particles in the simulation were not affected.

### Interactions

Several types of interactions can be defined between particles, the following were used in the existing model:

- 1) Coulomb interactions.
- 2) Lennard-Jones interactions (Circle).
- 3) Morse interaction.
- 4) Harmonic bending interaction ( $\theta$ ).
- 5) Harmonic stretch interaction ( $l$ ).

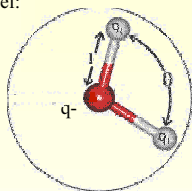
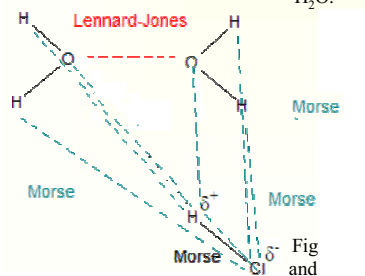


Figure 2. Bend, Stretch, Coulomb and Lennard-Jones interactions of  $H_2O$ .



Morse, Lennard-Jones mb interactions.

### Model Interactions

The Lennard-Jones interaction accounts for the size of the water molecules. It is repulsive at short distances, ensuring that the structure does not completely collide due to the electrostatic interactions. At intermediate distances it is attractive.

The Morse interaction is a potential that describes the same sorts of interactions as the Lennard-Jones potential. Morse interactions however, have an extra parameter, which means that Morse interaction can be adjusted to approach reality more readily than Lennard-Jones interaction.

## Results

After a few calculations were run, using the model, the following results were found:

- 1) The HCl molecule did *not* dissociate in the standard model.
- 2) With a dissociation energy 3.5 times as small as the original, the HCl *did* dissociate.
- 3) Reduction of negative charge to neutral in Cl ( $-0.9$  and  $0$ ) did not lead to dissociation. However, the arrangement of water molecules around the HCl did more closely resemble reality.
- 4) Using a larger box and thereby a lower concentration did not have an effect on the dissociation of HCl.
- 5) Raising the temperature ( $350$  K and  $400$  K instead of  $293$  K) did not have any noticeable effect on the dissociation of HCl.

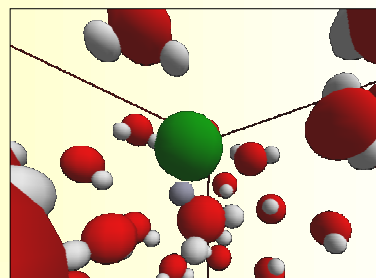


Figure 4. Dissociated HCl molecule  $Cl^-$  and  $H_3O^+$ .

## Discussion

The dissociation energy used in the original model had to be changed to a lower value, because the force constant for HCl as a gas was used instead of the force constant for HCl (aq).

## Conclusion

The HCl molecule dissociates when the Morse dissociation energy is lowered. This was expected because the value used in the original input was for HCl in gaseous phase.

## References

- [1] D.M. Ferguson; J. Comp. Chem., Vol 16, No. 4, 501-511, Parameterization and Evaluation of a flexible water model
- [2] H.J.C. Berendsen et al.; J. Chem. Phys. 81 (8), 15 October 1984, Molecular dynamics with coupling to an external bath