

## Abstract

This summer we simulated the potential of a methane molecule in a solution of water. We did this in multiple ways. The two most important ways were by using the Lennard Jones potential that is built into GROMACS to see how the radial distribution function should behave. From there we created a user defined function and a user table that allowed us to manually alter the interactions between certain molecules. The potential function can be split up into a dispersion force, C, a short range repulsive force, A, and an electrostatic force, Q. We set Q equal to zero and kept A constant at A=1. Then, using the table we created, we were able to vary the value of C to determine how the attractive force modified the potential through the radial distribution function (RDF). We found that as we increased C, the peaks of the RDF became more pronounced. From there, by performing more simulations and continuing to research this phenomena, we will be able to determine whether the potential is linearly dependent, non-linearly dependent, or independent of C

## Introduction

### Aim:

To create a user specified function in GROMACS that investigates the correlations of the potential function between a solute and water.

### Potential Function:

$$V(r) = \frac{qiqj}{4\pi\epsilon_0} f(r) + Cg(r) + Ah(r)$$

Inter molecular interactions between atoms split into three parts:

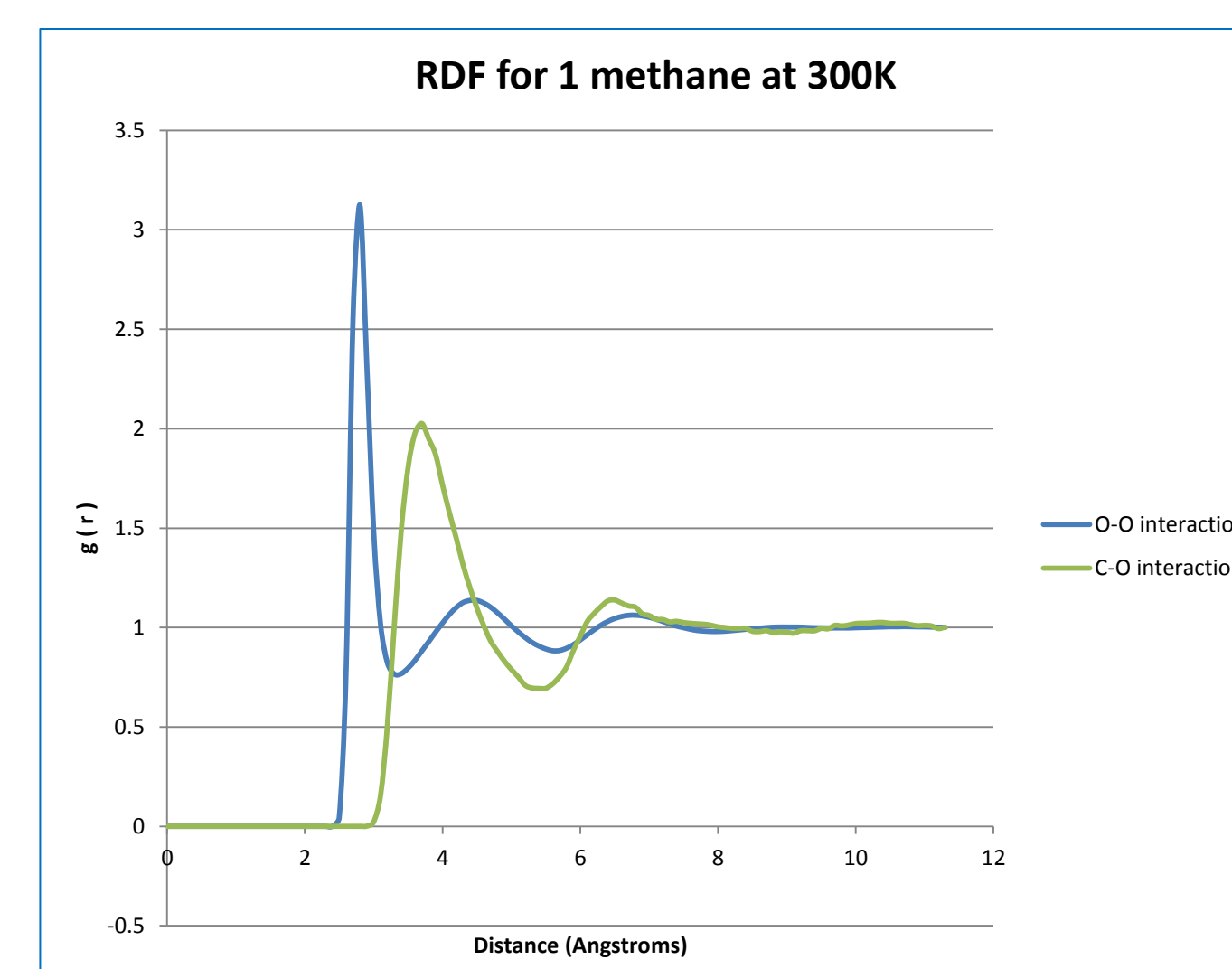
- Electrostatic interaction
- Dispersion Interaction
- Short range repulsion

GROMACS has a built in functions that allow either Lennard Jones 12-6 potential or Buckingham interactions, but does not explicitly allow for custom non-bonded interactions.

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## Methods: Computer Analysis

- First we used the built in potential simulation
  - PuTTY
    - Implementation of Telnet and SSH for Windows and Unix platforms
- GROMACS
  - GRoningen Machine for Chemical Simulations
  - Created methane molecule using Amber 8
  - Inserted single methane into solution of 400 water molecules
    - Ran simulation to equilibrium for 2 nanoseconds
    - Continued simulation in a production run of 10 nanoseconds

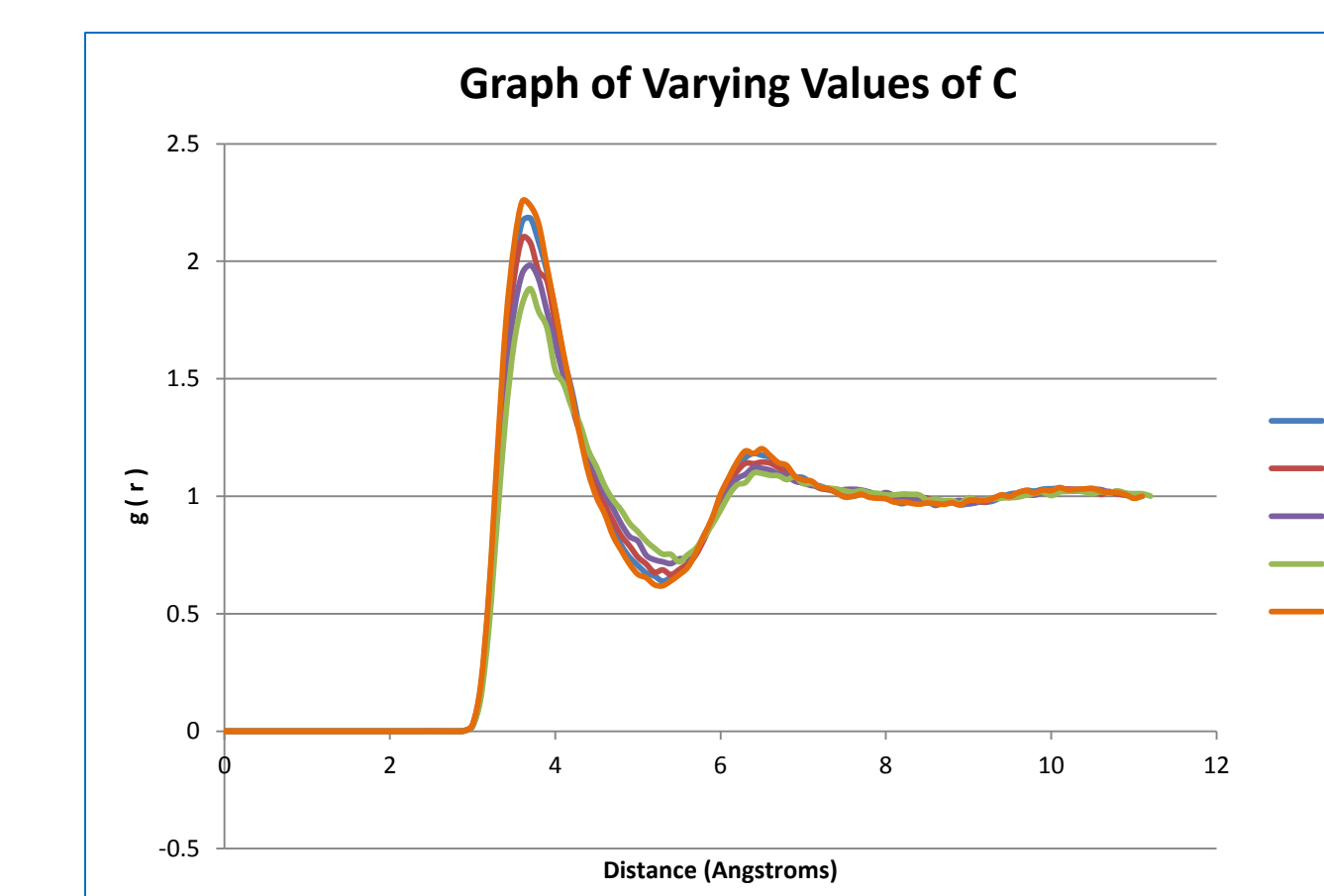


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## Methods: User Analysis

- Modified the topology file and amber files to allow for table input
- Created table that accounted for varying values of f(r), g(r), and h(r).
  - Set the parameters for A and C as
 
$$A = 4\epsilon\sigma^{12}$$

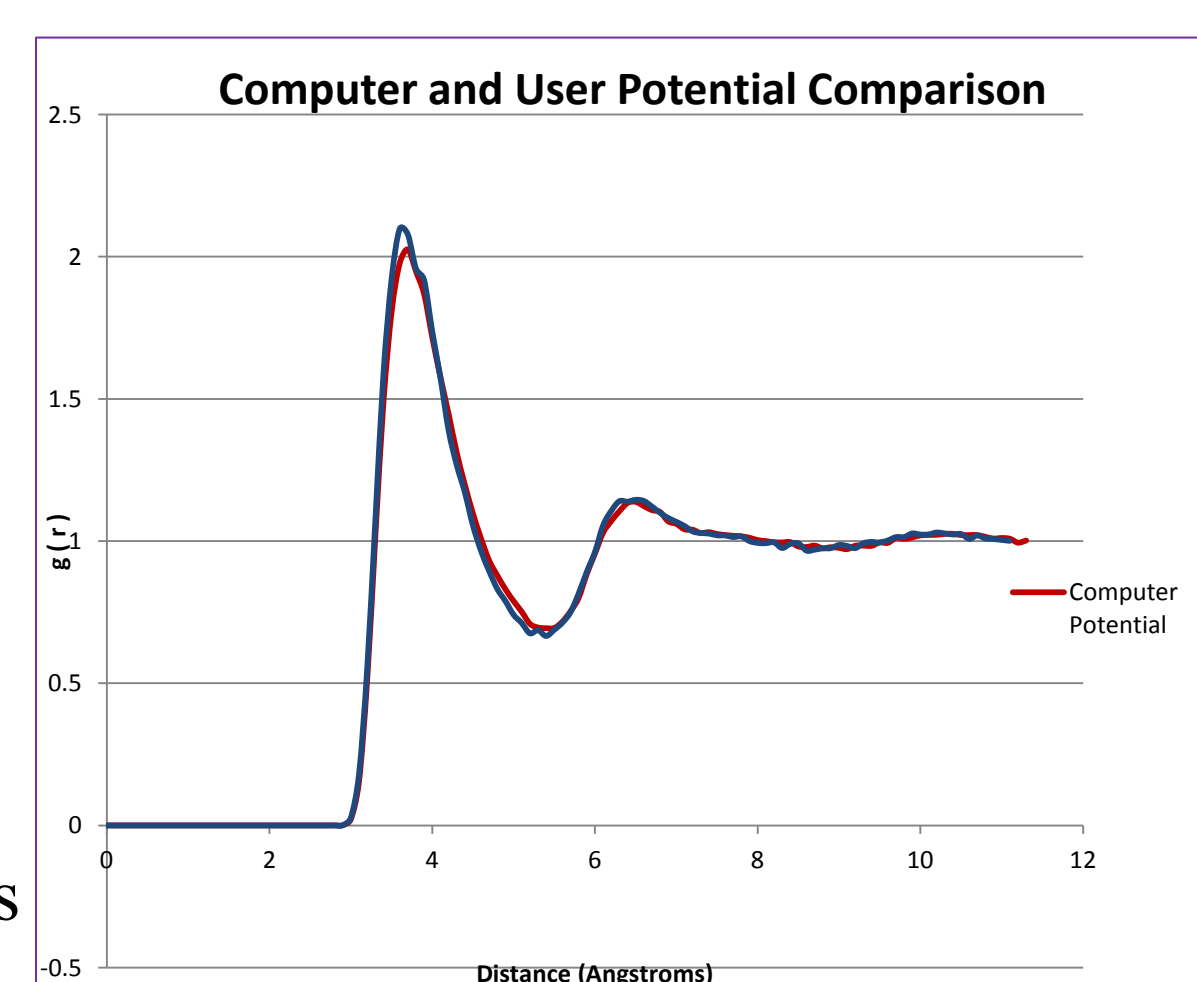
$$C = 4\epsilon\sigma^6$$
  - And set
 
$$\frac{qiqj}{4\pi\epsilon_0} = 0$$
- Set A=1 and C=1 to compare with data from the computer analysis
- Varied C while keeping A constant
  - C=[0,2] in increments of .5
  - A=1
- Created charts of RDFs for all values of C
  - Interactions between Carbon and Oxygen



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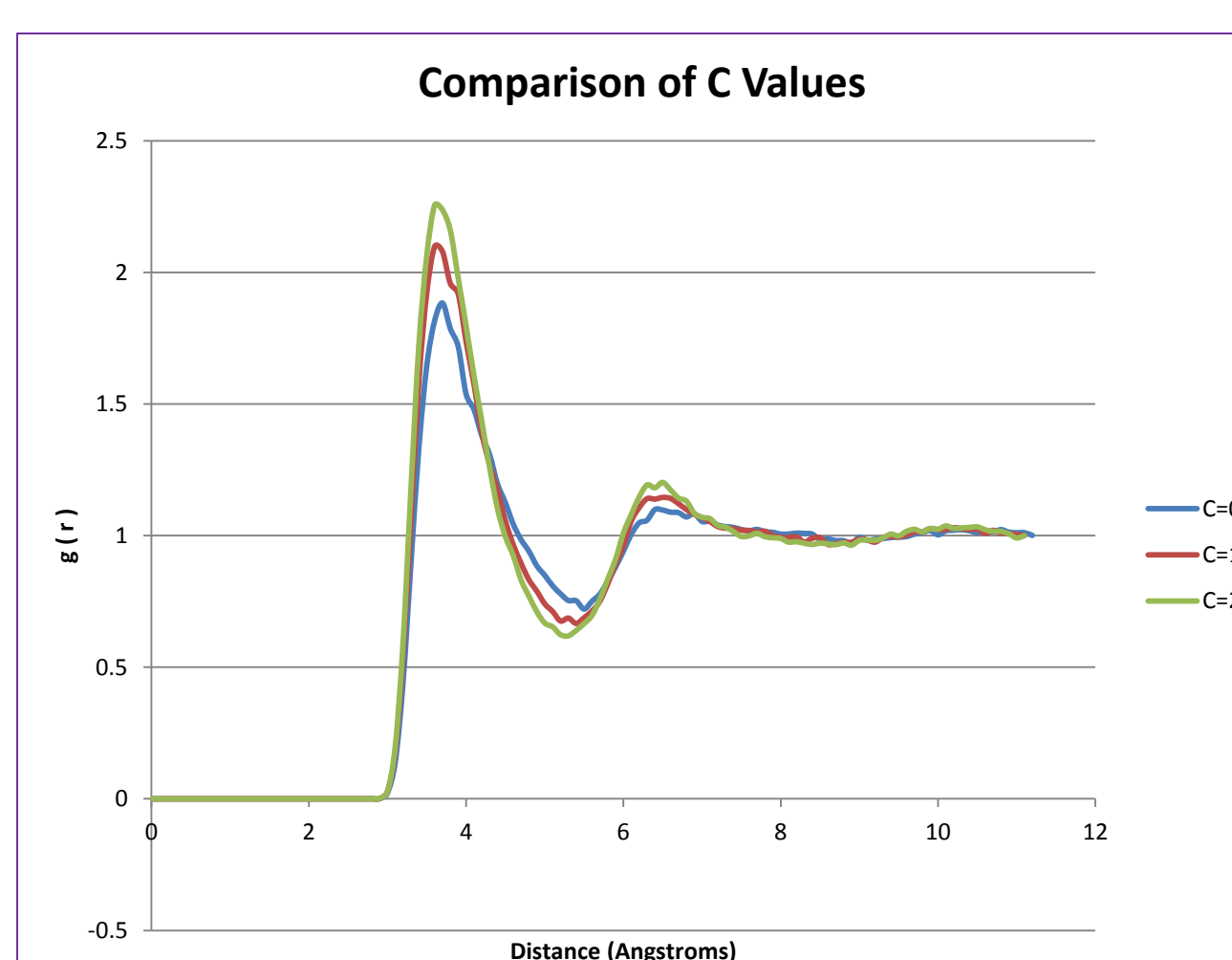
## Results and Discussion

User specified potential agreed with potential simulated by built in GROMACS functions



As C varies, the RDF graph varies with changes in the magnitude of the dispersion interaction

As C increases, the amplitude of the peaks on the carbon-oxygen RDF increased

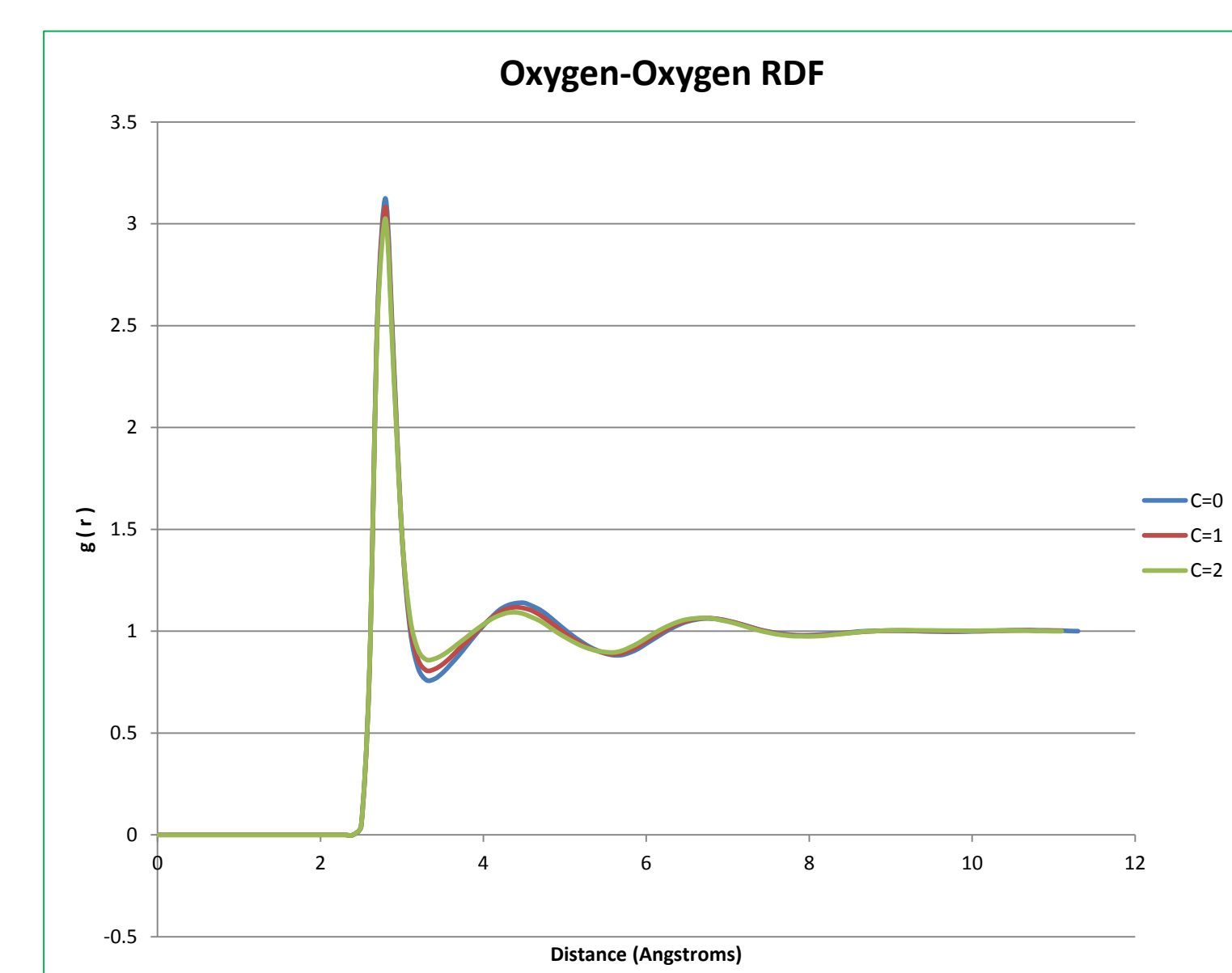


As C increased, the amplitude of the peaks on the oxygen-oxygen RDF decreased

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## Conclusion and Future Work

- The graph of G(r) versus distance suggests that the non-bonded potential of methane and water is linearly dependent on changes in the dispersion interaction
- Increasing the attraction between oxygen molecules decreased the distance between molecules as expected



- Further research into the relationship between the density fluctuations and the correlation function between the solute and water
- Simulate the thermodynamic response of the RDF to C
- More research required to see if the potential can be shown statistically to be linearly dependent upon changes in C
  - Might be linear on a small scale but not linear over all

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## References

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