Technical Manuscript Writing for Doctoral Candidates

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Module 11. The Results and Discussion Section

I. Parts of the Results and Discussion Section

Depending on the type of research being reported, the results and discussion section typically perform several important functions:

- presenting results
- explaining results
- comparing results to existing work, and explaining disagreements
- describing the implications and significance of the work

Let us review the Results and Discussion portion of the outline for each of the two study manuscripts. These portions are copied from the module on outlines (Module 3).

Example 1. A Theoretical Manuscript

[Wang *et al.*, *Phys. Rev. E* **81** 061204 (2010)]

IV. Results

- IV.A. Simple fluid monatomic molecule
  - IV.A.1. Compare PCFs for the monatomic system from MD and OZPY (¶ 20, p 5)
  - IV.A.2. Report the PCFs for the monatomic system from OZPY (¶ 21, p 5)
  - IV.A.3. Report the CG potentials (¶ 22, p 5)
  - IV.A.4. Examine failure of approximate equation 1 (¶ 23, p 5)
  - IV.A.5. Report the cavity function (¶ 24, p 6)
- IV.B. Diatomic fluid at low density
  - IV.B.1. Report the diatomic low density RDFs (¶ 25, p 6)
  - IV.B.2. Report the diatomic low density CG potential (¶ 26, p 7)
- IV.C. Diatomic fluid at high density
  - IV.C.1. Report the diatomic high density RDFs (¶ 27, p 7)
  - IV.C.2. List Potential Sources of Error (¶ 28, p 7)
  - IV.C.3. Evaluate Likelihood of Various Sources of Error (¶ 29, p 7)
  - IV.C.4. Fit conventional potential to CG potential (¶ 30, p 8)
  - IV.C.5. Discuss potential for future applications (¶ 31, p 8)

Example 2. An Experimental Manuscript

[Liu *et al.*, *Chem. Eng. J.* **151** pp. 235-240 (2009)]

3. Results and discussion

- 3.1. Preparation and characterization of the particles
  - 3.1.1. Comparison of structure of composite and Fe_3O_4 particles (¶ 9, p 2)
  - 3.1.2. Report water content (¶ 10, p 2)
  - 3.1.3. Report PZC results (¶ 11, p 2)
- 3.2. Adsorption kinetic curves (¶ 12, p 2)
- 3.3. Effect of initial solution pH on Adsorption (¶ 13, p 3)
- 3.4. Effect of ionic strength on the adsorption (¶ 14, p 3)
- 3.5. Adsorption mechanisms
  - 3.5.1. Expectations for differences in adsorption (¶ 15, p 3)
  - 3.5.2. Present proof that complexation is not responsible for adsorption (¶ 16, p 4)
  - 3.5.3. Form of boron present in the solutions of this work (¶ 17, p 4)
  - 3.5.4. Confirmation of the importance of electrostatic interactions (¶ 18, p 4)
  - 3.5.5. Report adsorption vs ionic strength (¶ 19, p 4)
  - 3.5.6. Role of hydrogen bonding (¶ 20, p 4)
  - 3.5.7. Role of hydrophobic interacations (¶ 21, p 4)
  - 3.5.8. Summary of three types of interactions (¶ 22, p 5)
  - 3.5.9. Three regimes of adsorption (¶ 23, p 5)
  - 3.5.10. Adsorption of both anion and neutral species occurs (¶ 24, p 5)

We examine below how this structure of the Results and Discussion section accomplishes the five tasks listed above.

II. Contents of the Results and Discussion Section

II.A. Presenting, Explaining and Comparing Results

The Results and Discussion section is where the results of the work are presented. These paragraphs typically have a standard formula.

- a statement of what is being presented
- a statement of the most important trends in the data
- an explanation of this trends
- a statement of the more subtle trends in the data
- an explanation of these trends
- other notes and clarifications
- comparison with existing work*

*If there is a short comparison with other published experiment or theory, then that short comparison can be included in this paragraph. If it is a lengthy comparison, then it may be better to include it as a separate paragraph.

Let’s consider a couple examples.

Example 1. An Experimental Manuscript

[Liu *et al.*, *Chem. Eng. J.* **151** pp. 235-240 (2009)]

Fig. 4 shows the amount of adsorbed boron as a function of time. As shown in Fig. 4, adsorption occurs rapidly in the first 2 h, after which the adsorption amount changes slowly. The particle composition does not have a significant effect on the equilibrium time. The variation in the extent of the adsorption may be because initially all sites on the surfaces of the particles were vacant and the boron concentration gradient was relatively high. Consequently, the extent of each ion uptake decreases significantly with the increase of contact time, caused by the decrease in the number of vacant sites on the surface of the particles. According to the adsorption kinetic results, the adsorption time was fixed at 2 d in the following experiments to make sure that the equilibrium was reached.

- a statement of what is being presented

Fig. 4 shows the amount of adsorbed boron as a function of time.

- a statement of the most important trends in the data

As shown in Fig. 4, adsorption occurs rapidly in the first 2 h, after which the adsorption amount changes slowly.

The particle composition does not have a significant effect on the equilibrium time.

- an explanation of this trend

The variation in the extent of the adsorption may be because initially all sites on the surfaces of the particles were vacant and the boron concentration gradient was relatively high. Consequently, the extent of each ion uptake decreases significantly with the increase of contact time, caused by the decrease in the number of vacant sites on the surface of the particles.

- other notes and clarifications

According to the adsorption kinetic results, the adsorption time was fixed at 2 d in the following experiments to make sure that the equilibrium was reached.

Example 2. A Simulation Manuscript

[Esai Selvan *et al.*, *Molec. Simul.* **36**(7-8) pp. 568–578 (2010)]

The distribution profiles of water molecules in confined geometries have been widely studied [56–58]. Figure 3(a) represents the density profile of water in a non-reactive system along the radial distance for different channel radii. The density near the CNT wall decreases with the channel radius. The number of peaks in the radial density profile increases as the CNT radius increases, implying the increase in water layers within the tube. At larger CNT radii, the density near the centre of the tube approaches the bulk water density, which indicates that as the *channel radius increases we find bulk water behaviour towards the centre of the tube where the fluid–tube interaction is weak. In other works, where the CNTs are modelled atomistically both ordered structures (helical [59] or n-gonal rings [60], where n is based on the radius) and organised layers were observed depending on the geometry of the CNT, pressure, temperature, water model and many other simulation parameters.*

- introductory sentence

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- a statement of what is being presented

Figure 3(a) represents the density profile of water in a non-reactive system along the radial distance for different channel radii.

- a statement of the most important trends in the data

The density near the CNT wall decreases with the channel radius. The number of peaks in the radial density profile increases as the CNT radius increases,

- an explanation of this trends

implying the increase in water layers within the tube.

- a statement of the more subtle trends in the data

At larger CNT radii, the density near the centre of the tube approaches the bulk water density,

- an explanation of these trends

which indicates that as the channel radius increases we find bulk water behaviour towards the centre of the tube where the fluid–tube interaction is weak.

- comparison with existing work*

In other works, where the CNTs are modelled atomistically both ordered structures (helical [59] or n-gonal rings [60], where n is based on the radius) and organised layers were observed depending on the geometry of the CNT, pressure, temperature, water model and many other simulation parameters.

Example 3. A Theoretical Manuscript

[Wang *et al.*, *Phys. Rev. E* **81** 061204 (2010)]

These PCFs were input into the OZPY−1 procedure to obtain the interaction potentials. The interaction potentials are compared with the original Lennard-Jones 12-6 potential in Fig. 5.

The potentials are shifted by increments of 0.25 on the y axis for clarity. As expected, excellent agreement is shown in Fig. 5 for low-density cases. As the density increases there is a small but growing discrepancy between the original potential and the potential from the OZPY−1 procedure, which we attribute to numerical approximations in the evaluation of the integrals. This source of error was confirmed by increasing the size of the discretization and observing that the noise in the data also increased. Generally, we see that the OZPY−1 procedure is able to satisfactorily reproduce the interaction potential.

- introductory statement, linking the next figure to the previous figure

These PCFs were input into the OZPY^{-1} *procedure to obtain the interaction potentials.*

- a statement of what is being presented

The interaction potentials are compared with the original Lennard-Jones 12-6 potential in Fig. 5. The potentials are shifted by increments of 0.25 on the y axis for clarity.

- a statement of the most important trends in the data

As expected, excellent agreement is shown in Fig. 5 for low-density cases.

- an explanation of this trends

None necessary, since this is the expected behavior.

- a statement of the more subtle trends in the data

As the density increases there is a small but growing discrepancy between the original potential and the potential from the OZPY^{-1} *procedure,*

- an explanation of these trends

which we attribute to numerical approximations in the evaluation of the integrals. This source of error was confirmed by increasing the size of the discretization and observing that the noise in the data also increased. Generally, we see that the OZPY^{-1} *procedure is able to satisfactorily reproduce the interaction potential.*

II.B. Discussing Results

Discussions are more than simply presenting results. There can be extensive comparison with published data, either comparable work of others, or the comparison of experimental work with theoretical predictions (or vice versa). The discussion section also provides the opportunity to discuss the broader significance of the work.

Again, let us look at some examples.

Example 4. An Experimental Manuscript

[Liu *et al.*, *Chem. Eng. J.* **151** pp. 235-240 (2009)]

In this manuscript, the first four sub-sections of the Results and Discussion section present Results. The last sub-section, *3.5. Adsorption mechanisms*, present a discussion. The purpose of this discussion is to analyze all of the data together and come up with a molecular-level description of the adsorption process.

Let us examine this sub-section in the manuscript. We do not reproduce it here in the notes.

Example 5. A Simulation Manuscript

[Esai Selvan *et al.*, *Molec. Simul.* **36**(7-8) pp. 568–578 (2010)]

In the paragraph reproduced, below, the impact of confinement on the transport of charge in carbon nanotubes (CNT) is illustrated by comparison to the same values in bulk water.

A better way to understand the effect of confinement on the charge diffusion would be to compare these diffusivity values to that of bulk water from our previous work. The total, structural and vehicular diffusivities of proton in bulk water at 300 K are $7.33x10^{-5}$, $4.29x10^{-5}$ *and* $2.83x10^{-5}$ cm^2/s *based on our algorithm [14]. When we compare these values to the CNT with the largest radius, we find that the vehicular diffusivities are virtually the same while the structural component is only 12% of the value observed in bulk water. This can be explained by the obvious reduction in the rate constant. So, in overall, there is 58% reduction in the total charge diffusion at our largest CNT due to confinement.*

In the paragraph reproduced below, we compare our results with other simulation results, since there is no experimental data available.

Proton transport in confined water has been previously studied. The mobility of proton was much higher [34,37] in 1D water wires in armchair (6,6) CNTs (radius = 4.07 Å) than observed in bulk water. However, in cylindrical channels with 3D water structure, the proton diffusivity was computed to be much lower than that observed in bulk water but increased with channel diameter [36]. The centre of excess charge diffusion coefficient in a cylindrical channel of carbon with radius and length of 5 and 29.8 Å , respectively, containing 77 water molecules was about $2.5x10^{-5}$ cm^2/s *[36] compared to the computed value of 4.5 ^* $1.1x10^{-5}$ cm^2/s *in bulk water using the MS-EVB model. The charge diffusivity at our smallest CNT of radius 5.42 Å is* $1.30x10^{-5}$ cm^2/s *compared to the value of* $7.33x10^{-5}$ cm^2/s *in bulk water. Therefore, we observe the same qualitative trend with the RMD algorithm as is observed with the MS-EVB model.*

Example 6. A Theoretical Manuscript

[Wang *et al.*, *Phys. Rev. E* **81** 061204 (2010)]

When it clear that there is a discrepancy, an extended error analysis, in which one searches for the source of the error by investigating various possibilities can be included in the discussion. An example of this discussion is given below.

We now discuss the possible sources of error and their impact. A potential source of error is that we have assumed that Eq. _1_ is true for the stretching potential. Equation _1_ implies the stretching distribution is independent of the nonbonded distribution. This error can be determined to be small in this case since the stretching potential extracted from Eq._1_ matches the stretching potential used in the MD simulation.

The error could be due to the fact that the MD simulation and the OZPY description of the diatomic fluid are not the same. In other words, the error is a manifestation of the approximation in the integral equation theory. Such errors have been noted before. For example, using the hypernetted chain _HNC_ closure, Bresme et al. _13_ proved that the bond length and stretching interaction potential could affect the comparison of structural properties of diatomic Lennard-Jones fluids calculated by OZ integral theory with simulation data. This is because solving the OZ integral with HNC closure using a central force model cannot satisfy the condition that the number of bonds per atom is unity, compared with the real diatomic Lennard-Jones fluid. In our inverse procedure, we used the PCFs from MD simulation of the Lennard- Jones fluid and we carefully checked the above-mentioned condition by integrating the PCFs over space. The average number of bonds per atom is about 1.05 for both low- and high-density cases. _The error is due to the small number of points in which the stretching distribution is nonzero and the approximate numerical integration._ So, while we do have the correct number of stretching modes per atom, we may still be subject to other impacts of the PY approximation_28_.