Technical Manuscript Writing for Doctoral Candidates

David J. Keffer
Department of Chemical and Biomolecular Engineering
Yonsei University
dkeffer@utk.edu

Module 12. The Conclusions Section

I. Parts of the Conclusions Section

The conclusions section typically perform several important functions:

- restates the purpose of the paper
- summarizes the most important results
- describes the broader impact of the work

Let us review the Conclusions portion of the outline for each of the two study manuscripts. These portions are copied from the module on outlines (Module 3). In each example, the conclusion is a single paragraph and is characterized by only one entry in the outline.

Example 1. A Theoretical Manuscript
[Wang *et al.*, *Phys. Rev. E* **81** 061204 (2010)]

V. Conclusions (¶ 32, p 8)

Example 2. An Experimental Manuscript
[Liu *et al.*, *Chem. Eng. J.* **151** pp. 235-240 (2009)]

4. Conclusion (¶ 25, p 5)

II. Contents of the Results and Discussion Section

II.A. Restatement of the Purpose of the Papers

Typically, the beginning of the conclusion contains a restatement of the purpose of the paper. In both of the examples that follow, the first sentence of the conclusions is a restatement of the purpose.

Example 1. A Theoretical Manuscript
[Wang *et al.*, *Phys. Rev. E* **81** 061204 (2010)]

We have demonstrated that the OZPY equation can be used to extract interaction potentials given distribution functions for monatomic and diatomic fluids.

Example 2. An Experimental Manuscript
[Liu *et al.*, *Chem. Eng. J.* **151** pp. 235-240 (2009)]

Pure Fe3O4 particles and two kinds of composite Fe3O4 particles were used to adsorb boron from aqueous solution.

II.B. Summary of the Results

The bulk of the conclusions section is a summary of the results. A list of major results should be included. The results need to be organized according to the same structure in which the paper was organized. You do not want a random collection of observations from the paper. You may want to refer back to your outline to make sure that you include a complete list of results for each part of the paper. Also, you should not include any new information in the conclusions section. The conclusions should simply be a summary of material that was already presented.

Example 1. A Theoretical Manuscript
[Wang *et al.*, *Phys. Rev. E* **81** 061204 (2010)]

monatomic gas results

In the monatomic fluid case, the procedure is able to reliably reproduce the original Lennard-Jones 12-6 potential up to moderate densities.

diatomic gas procedure

In the diatomic case, we first obtained the density distributions for stretching and nonbonded interaction sites from classical equilibrium MD simulation of nitrogen under lowand high-density cases.

diatomic gas low density results

By incorporating the stretching potential into the OZPY equation, we extracted a nonbonded interaction potential which matched the original Lennard-Jones 12-6 potential at low densities.

diatomic gas high density results

At higher densities, there was a systematic difference between the original potential and that extracted from the OZPY−1 procedure, which we attribute to the PY approximation.

However, the short-range portion of the potential is reproduced sufficiently well that the s and e parameters can be reproduced to within 1.1% and 1.0%, respectively.

Example 2. An Experimental Manuscript
[Liu *et al.*, *Chem. Eng. J.* **151** pp. 235-240 (2009)]

Observations from rate of boron adsorption

Boron adsorption occurred rapidly in the first 2 h and the effect of particle composition was negligible for the equilibrium time.

Effect of pH and solution composition on boron adsorption

We found that boron adsorption decreased with the initial pH in the order of 6.0 > 2.2 > 11.7 for all particles, and that at the same solution composition it decreased in the order of Fe3O4–TSPA> Fe3O4–1010f > Fe3O4 particles.

Effect of ionic strength on boron adsorption

In general, the adsorption amount decreased with the increase in ionic strength.

Summary of mechanism

It was suggested that boron is adsorbed in both forms of H3BO3 and B(OH)4−. Thus, for all the particles the amount of boron adsorption is highest in neutral solution probably due to the hydrogen bonding, electrostatic and hydrophobic attractions, but lowest in basic solution because of the electrostatic repulsion.

II.C. Broader Impacts

The conclusions can end with a statement of the broader impacts and potentially areas for future research. The experimental manuscript does not contain a broader impacts statement.

Example 1. A Theoretical Manuscript
[Wang *et al.*, *Phys. Rev. E* **81** 061204 (2010)]

summary of the impact of the work

This level of accuracy would represent an improvement in the development of coarse-grained potentials.

future work

Application to polymeric systems is underway.