Technical Manuscript Writing for Doctoral Candidates

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Module 5. Figures and Tables

Introduction to Figures and Tables

Engineering is a quantitative field. We work report numbers and expect these numbers to convey some meaning to the reader. Thus figures and tables are an essential component of the technical manuscript. In this module we have two objectives" The first objective is to determine appropriate content for figures and tables. The second objective is to provide guidelines for the formatting of publication quality figures and tables.

Determination of Content for Figures and Tables

You cannot report all of the raw data in your lab notebook in the technical manuscript. It is up to the authors to make the critical decisions regarding which information is of sufficient importance to present in graphical or tabular form in the manuscript. This is often a difficult decision. The decision has been made somewhat easier by the arrival of the internet, which has created an almost infinite capacity for "Supplementary Information" files. As mentioned earlier, supplementary information files are documents that contain supporting information that will never appear in the paper version of the journal. It is available (typically free of charge) on the internet. It must be included as part of the package that is submitted to the journal for review.

Example 1.

Let's look at a relatively famous example. The landmark paper for the synthesis of Metal Organic Frameworks (MOFs) appeared in Science[1]. The article itself is less than <u>four</u> pages and contains 3 Figures. The first figure is a schematic of the structure of the MOF. The second figure gives information regarding its structural characterization. The third figure provides information regarding its adsorptive capacity. In order to access the 4 page document, one must be at a university that is paying the subscription fee for the journal.

The accompanying supplementary information is <u>110</u> pages long. It contains the elemental analysis, the IR spectra, detailed sorption data, and all of the x-ray diffraction data that was used to determine crystallographic structure of the MOFs. In order to access the 110-page supplementary information document, one can simply go to the Science website and download the pdf file free of charge.

This example illustrates that one must be very selective in determining what information is worth including in the manuscript.

Determination of the Number of Figures and Tables

Editors want to limit the number of pages per article. If a manuscript includes too many figures, they will frequently request that the authors reduce the number of figures, with the option of moving some of them to the supplementary information document. Most papers do not include a supplementary information document, so there is a real challenge in selecting the most important figures and tables.

The figures and tables must satisfy several criteria.

(1) Every figure and table must convey important information.
(2) Every figure and table must convey unique information.
(3) Every figure and table must be discussed in the text.
(4) Every figure and table must be easily understood.

The first three of these criteria have to do with the selection of figures and tables. The last has to do with formatting. Because of the first two criteria, Figures are tied to the outline. If you can't find a place in the outline that corresponds to the figure, then the figure doesn't belong in the manuscript. Let's return to our two study manuscripts.

Example 2. Figures in a Theoretical Manuscript

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

We reproduce the detailed outline of this manuscript, as was first presented in Lecture Module 2. This time we also highlight where each Figure belongs.

Figure 1 is a schematic showing the procedure that corresponds to the purpose of the paper. Figure 1 is discussed in section I.C. Restatement of purpose of paper (¶ 11, p 2).

Figure 2 is a schematic showing the allowable diatomic interactions. Figure 2 is discussed in section III.C. Adaptation of the OZ equation for diatomic molecules, example (¶ 16, p 3) .

Figure 3 is a result discussed in IV.A.1. Compare PCFs for the monatomic system from MD and OZPY (¶ 20, p 5)..

Figure 4 is a result discussed in IV.A.2. Report the PCFs for the monatomic system from OZPY (¶ 21, p 5).

Figure 5 is a result discussed in IV.A.3. Report the CG potentials (¶ 22, p 5).

Figure 6 is a result discussed in IV.A.4. Examine failure of approximate equation 1 (¶ 23, p 5).

Figure 7 is a result discussed in IV.A.5. Report the cavity function (¶ 24, p 6).

Figure 8 is a result discussed in IV.B.1. Report the diatomic low density RDFs (¶ 25, p 6).

Figure 9 is a result discussed in IV.B.2. Report the diatomic low density CG potential (¶ 26, p 7).

Figures 10 & 11 are results discussed in IV.C.1. Report the diatomic high density RDFs (¶ 27, p 7).

Table 1 is a tabular form of Figure 2 and is discussed in III.C. Adaptation of the OZ equation for diatomic molecules, example (¶ 16, p 3).

Detailed Outline: Wang *et al.*, *Phys. Rev. E* **81** 061204 (2010)

0. abstract

I. Introduction

- I.A. Background on Generating Coarse-Grained (CG) Potentials
  - I.A.1. Procedure for Generating CG Stretching/Bending Potentials (¶ 1, p 1)
  - I.A.2. This Procedure is inadequate for Non-bonded Potentials (¶ 2, p 1)
  - I.A.3. Existing Procedure #1 for Generating CG Non-bonded Potentials (¶ 3, p 1)
  - I.A.4. Existing Procedure #2 for Generating CG Non-bonded Potentials (¶ 4, p 1)
- I.B. Review of the Literature: The Orstein-Zernike Percus-Yevick (OZPY) integral equation
  - I.B.1. Introduction to OZPY (¶ 5, p 2)
  - I.B.2. Typical uses of OZPY (¶ 6, p 2)
  - I.B.3. Application of OZPY to simple fluids (¶ 7, p 2)
  - I.B.4. Application of OZPY to polymers (¶ 8, p 2)
  - I.B.5. Application of inverse OZPY to polymers (¶ 9, p 2)
  - I.B.6. Advantages of inverse OZPY approach (¶ 10, p 2)
- I.C. Restatement of purpose of paper (¶ 11, p 2) Fig. 1.

II. Simulation

- II.A. Numerical Method for Monatomic Fluid Simulations (¶ 12, p 2)
- II.B. Numerical Method for Diatomic Fluid Simulations (¶ 13, p 3)

III. Theory

- III.A. Definition of the OZ equation (¶ 14, p 3)
- III.B. Adaptation of the OZ equation for diatomic molecules (¶ 15, p 3)
- III.C. Adaptation of the OZ equation for diatomic molecules, example (¶ 16, p 3) Fig. 2. & Table 1.
- III.D. Derivation of the OZPY equation (¶ 17, p 4)
- III.E. Recast OZPY equation in terms of density distributions rather than PCFs (¶ 18, p 4)
- III.F. Notes on numerical evaluation of theory (¶ 19, p 5)

IV. Results

- IV.A. Simple fluid monatomic molecule
  - IV.A.1. Compare PCFs for the monatomic system from MD and OZPY (¶ 20, p 5) Fig. 3.
  - IV.A.2. Report the PCFs for the monatomic system from OZPY (¶ 21, p 5) Fig. 4.
  - IV.A.3. Report the CG potentials (¶ 22, p 5) Fig. 5.
  - IV.A.4. Examine failure of approximate equation 1 (¶ 23, p 5) Fig. 6.
  - IV.A.5. Report the cavity function (¶ 24, p 6) Fig. 7.
- IV.B. Diatomic fluid at low density
  - IV.B.1. Report the diatomic low density RDFs (¶ 25, p 6) Fig. 8.
  - IV.B.2. Report the diatomic low density CG potential (¶ 26, p 7) Fig. 9.
- IV.C. Diatomic fluid at high density
  - IV.C.1. Report the diatomic high density RDFs (¶ 27, p 7) Figs. 10 & 11.
  - 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)

V. Conclusions (¶ 32, p 8)

VI. Acknowledgments (¶ 33, p 8)

VII. References

This example illustrates several points.

(1) Every figure and table must convey important information.
(2) Every figure and table must convey unique information.
(3) Every figure and table must be discussed in the text.

Example 3. Figures in an Experimental Manuscript

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

We reproduce the detailed outline of this manuscript, as was first presented in Lecture Module 2. This time we also highlight where each Figure belongs.

Figure 1 is a schematic showing the reactions and is discussed in 3.1.1. Comparison of structure of composite and Fe_3O_4 particles (¶ 9, p 2).

Figure 2 is a result discussed in 3.1.1. Comparison of structure of composite and Fe_3O_4 particles (¶ 9, p 2).

Figure 3 is a result discussed in 3.1.3. Report PZC results (¶ 11, p 2) ..

Figure 4 is a result discussed in 3.2. Adsorption kinetic curves (¶ 12, p 2).

Figure 5 is a result discussed in 3.3. Effect of initial solution pH on Adsorption (¶ 13, p 3).

Figure 6 is a result discussed in 3.4. Effect of ionic strength on the adsorption (¶ 14, p 3).

Figure 7 is a schematic illustrating one of the important conclusions of the manuscript discussed in 3.5.8. Summary of three types of interactions (¶ 22, p 5).

This manuscript has no tables.

This example illustrates the same three points as the previous example.

(1) Every figure and table must convey important information.
(2) Every figure and table must convey unique information.
(3) Every figure and table must be discussed in the text.

Detailed Outline: Liu *et al.*, *Chem. Eng. J.* **151** pp. 235-240 (2009)

0. abstract

1. Introduction
   1.1. Background on Boron (¶ 1, p 1)
   1.2. Existing ways to remove boron from water (¶ 2, p 1)
   1.3. Introduce Magnetic Assisted Adsorption Separation (¶ 3, p 1)
   1.4. Restatement of purpose of paper (¶ 4, p 2)

2. Experimental
   2.1. Preparation of pure Fe_3O_4 particles and the composite magnetic particles
      2.1.1. Preparation Procedure (¶ 5, p 2)
      2.1.2. Equipment Information (¶ 6, p 2)
   2.2. Boron adsorption
      2.2.1. Adsorption Procedure (¶ 7, p 2)
      2.2.2. Separation Procedure (¶ 8, p 2)

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) Figs. 1 & 2.
      3.1.2. Report water content (¶ 10, p 2)
      3.1.3. Report PZC results (¶ 11, p 2) Fig. 3.
   3.2. Adsorption kinetic curves (¶ 12, p 2) Fig. 4.
   3.3. Effect of initial solution pH on Adsorption (¶ 13, p 3) Fig. 5.
   3.4. Effect of ionic strength on the adsorption (¶ 14, p 3) Fig. 6.
   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) Fig. 7.
      3.5.9. Three regimes of adsorption (¶ 23, p 5)
      3.5.10. Adsorption of both anion and neutral species occurs (¶ 24, p 5)

4. Conclusion (¶ 25, p 5)

5. Acknowledgments (¶ 26, p 5)
6. References

Example 4. Journals that Focus on Data

If the journal focuses on data, then the rules for figures and especially tables are different. Let us look at an example from the *Journal of Chemistry and Engineering Data*[2]. In this manuscript there are lengthy tables. Most journals would not publish tables like this. It is the purpose of the *Journal of Chemistry and Engineering Data* to present complete and precise tables of physical properties.

Example 5. Graphics Intensive Journals

Some journals focus on graphics and images. The rules for the number of figures that can appear in these journals are different. You must read the "Instructions for Authors" information on the journal website. Also you must examine several papers recently published in that journal to discern the appropriate number. As an example, let us look at a paper from the Journal of Molecular Graphics and Modeling [3]. This paper has numerous snapshots from simulation that provide visual evidence to support various conclusions of the simulation research. We should point out that this paper was the by-product of research generating quantitative data. In the end, we had so many beautiful graphics that helped visualize for example the molecular origin of shear thinning that we sought out the appropriate journal to publish these images.

More on Supplementary Information Documents

Editors want to limit the number of pages per article. If a manuscript includes too many figures, they will frequently request that the authors reduce the number of figures, with the option of moving some of them to the supplementary information document. Again, with the advent of Supplementary Information on the internet, this decision to just present the most important information in the manuscript becomes much easier. Let's look at an example.

Example 6.

In this example, we look at a recent paper modeling the use of MOFs to preconcentrate explosive molecules for sensing purposes[4].

The manuscript is 10 pages long and contains 10 figures and 4 tables. The first 3 figures convey the structure of the MOF and the explosive. Figures 4-8 are results including adsorption isotherms, binding energies, adsorption site locations, diffusivities and activation energies. Figures 9 & 10 report some of the similar results for a different set of charges used in the model. Note that not all of the figures are presented again for the second model. Only the most important that show some difference from that of the first model. The Tables in the manuscript present data on the MOF structures, Henry's Law Constants (slopes of the isotherms in Figure 4), binding energies and loadings for the second model.

The Supplementary Information document contains a derivation of the statistical mechanical adsorption model, 13 tables of data, and 3 additional figures. These tables include parameters used in the model as well as some additional results of the simulation. In some cases, the data that was presented in graphical form in the manuscript is also given in tabular form in the Supplementary information.

Warning: The Supplementary Information document cannot become a dumping ground for all kinds of data. It must be formatted and carefully written to the same standards as the published manuscript. It too is part of the archival process. It must be carefully assembled and include only valid information.

Formatting of Figures and Tables

The previous sections discussed determination of number and type of figures and tables. This section is strictly about making the figures and tables better able to convey their meaning to reader.

Basic Rules for Formatting Figures

Purpose:

The purpose of a data plot is to communicate to the reader the physical consequences of your data. Therefore, there are two ultimate goals of plot formatting. The first goal of plot formatting is to display your data HONESTLY (or objectively). Clever (and deceitful) or just plain careless manipulation of a plot can make data appear to support one hypothesis, when actually it supports another hypothesis. The second goal of plot formatting is to display your data with as much CLARITY as possible.

Guidelines:

I. Titles, axes, captions, legends, and text boxes

- In a technical paper, plots have no titles. Instead they have captions.
- The plot should have a simple, descriptive caption, which may contain additional information not given in the plot.
- The plot should have x and y-axes titles. If the x and y-axes have units, the units should be given.
- The range of the x and y axes should correspond to the data. There should not be large blank spaces in the plot.
- The x and y axes should have numerical values. The values should have only the minimum number of significant figures needed to convey to the reader the vicinity of the plot. For example, the numbers on the x-axis should be "0.1" and not "0.100".
- When displaying multiple data sets on the same figure, you need a legend. The legend should be short and sweet. In Figure One, we use the legend to distinguish between experimental and theoretical data.
- If, as in the case, of Figure One, there are some important parameters that are held constant for that plot, they should be stated in a blank space on the plot, if possible, and in the caption of the plot.

II. Plot content

- You should try to display as much related information on a single figure as possible, without compromising the clarity of the plot. Plotting data on the same figure, allows for ease of comparison. In Figure One, we plot both theory and experimental lines on the same plot. We could have plotted them on separate plots but that would have made it more difficult to compare the two. The two sets of data are still clearly displayed in Figure One and Two.
- In Figures Three and Four, six sets of data are clearly displayed. This allows us to see the coupled effect of the initial height and the pipe diameter. This is the best way to display the data, so long as the six data sets do not overlap to such a great extent that the plot becomes an unreadable jumble of lines.

III. Lines, curves, and markers ()

- Your plots should be honest. This means you should only display the data that you obtained. You have not measured how the system behaves between your data points. Therefore, you should not pretend that you know how the system behaves there. The only thing you know is what you measured.
- When displaying experimental data, you should use POINTS where you have a data points. You can connect the points with STRAIGHT lines, if you choose, for the sole purpose of guiding the reader's eye for clarity in the plot. You should never use a polynomial curve fit because you do not know how the experimental system behaves between your data points.
- If you want to show that data fits a certain model (e.g. linear or quadratic or exponential), you need to indicate that the line is a linear or quadratic or exponential best fit, in the legend. The coefficients of best fit in the model, should be given in the caption or the text of the report.
- When displaying an analytical theory, as is the case for theory 1 in Figures One and Three, you should use a smooth line without points. The analytical theory has been evaluated at many points. STRAIGHT lines between the points appear to the eye as curved. This is what has been done in Figures One and Three.
- Sometimes analytical theories require too much computational effort to evaluate at many data points. In this case the smooth theoretical curve in Figures One and Three cannot be obtained. In this case, we evaluate the theory at a few points. We then have "theory data points", which we must treat in precisely the same manner as "experimental data points". This means we use a marker at the data point and we connect with straight lines if we want to guide the reader's eye. This is what has been done in Figures Two and Four.
- In none of these plots did we connect the experimental points with a straight line. We could have, but we didn't need to because our eye was guided by the theoretical curve.
- In none of these plots did we use "curved" lines.

IV. Lines, curves, and markers (style)

- When displaying multiple data sets on the same figure, you should use different lines and points for the data. This is done in all four plots.
- In Figure Three, notice we used the same line for all three theoretical curves. We could have used a solid line, a dashed line, and a dotted line for the three theoretical curves. It is our choice. I did not use them because I believe the presence of the experimental data clearly distinguishes the theoretical data.
- In Figure Four, we have six sets of data. There are two variables in the data, theory vs. experiment and the initial water height. Notice how I have used open markers for all the experimental sets and filled markers with lines for the theoretical data sets. Note also that I have used the same markers for the same initial water heights. This tells the reader to compare open squares with filled squares, compare open triangles with filled triangles, compare open circles with filled circles, if they want to compare theory and experiment at the same value of initial water height. This also tells the reader to compare only open markers, if they want to look at experimental results as a

function of water height, or only filled markers, if they want to look at theoretical results as a function of water height.

- In Figure Four, I distinguished between theory sets by using different filled markers but the same style (solid) of line. There is no need to distinguish between data sets by changing both markers and lines.

V. Overall Plot Formatting

- Format all plots in a manuscript in the same way.
- Create a template and use it for all plots.
- Use the same font in all plots.
- Use the same aspect ratio for all plots. (The plots will look terrible if every aspect ratio is different, when the plots get grouped together on the journal page.)

VI. Color

Today, most journals still appear both in paper and in electronic form. If you make your figures in color, then they will appear in color in the electronic version, without any additional charge from the publisher. However, the publisher will generally charge you for figures that you want to appear in color in the paper version of the journal. Since it is unlikely that you will want to pay for color figures, the best plan is to not rely on colors in the figures. This is a good plan even if you are relying on the electronic version of the manuscript, because once the pdf file is printed on a black and white printer, any color information is lost.

Color, however, can often be beneficial to a plot, especially in quickly bringing differences to the eye. Thus, in an oral presentation or a poster, color figures are better than black and white figures. I frequently have students prepare two versions of the same figure—a color figure for oral presentations and posters and a black and white figure for the journal.

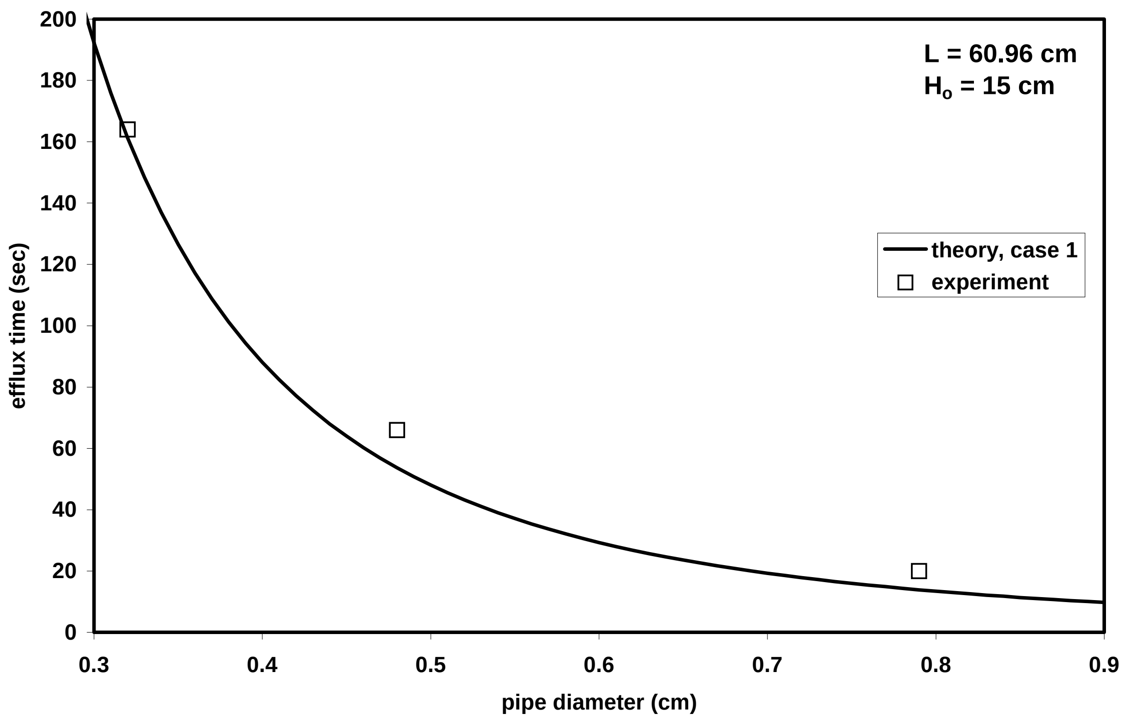

Figure One. Efflux time as a function of pipe diameter, using the pipe of Length 60.96 cm and an initial water height of 15 cm. The theory line represent Case One, equation (8).

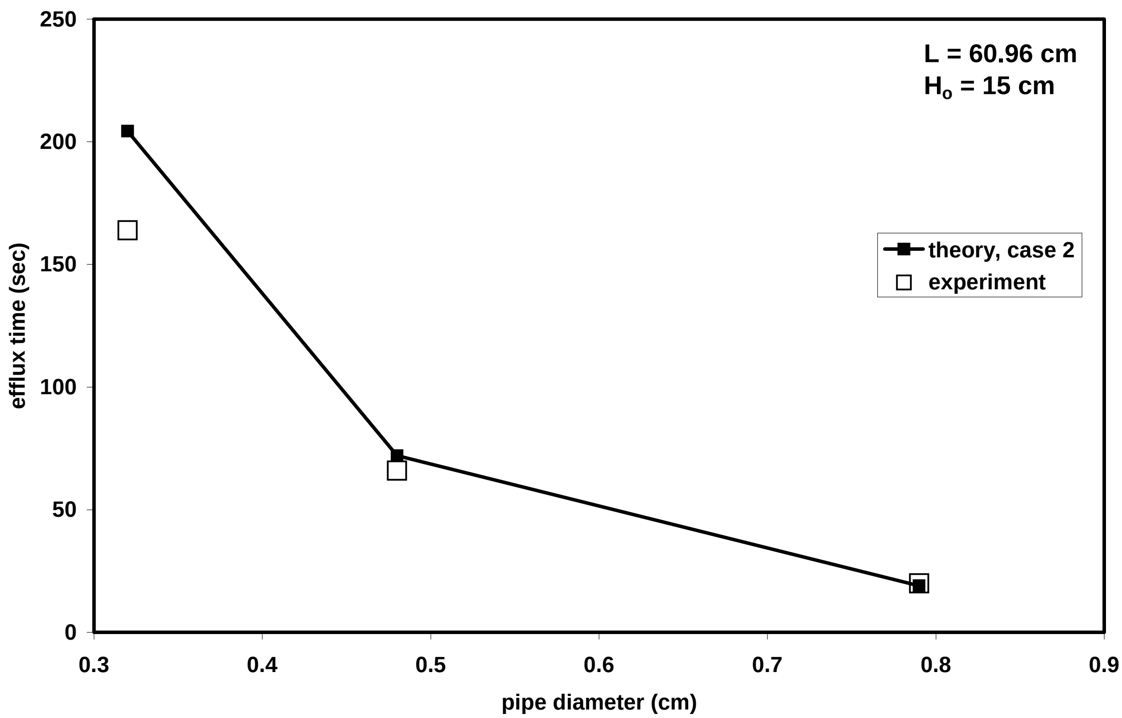

Figure Two. Efflux time as a function of pipe diameter, using the pipe of Length 60.96 cm and an initial water height of 15 cm. The theory line represent Case Two, equation (16).

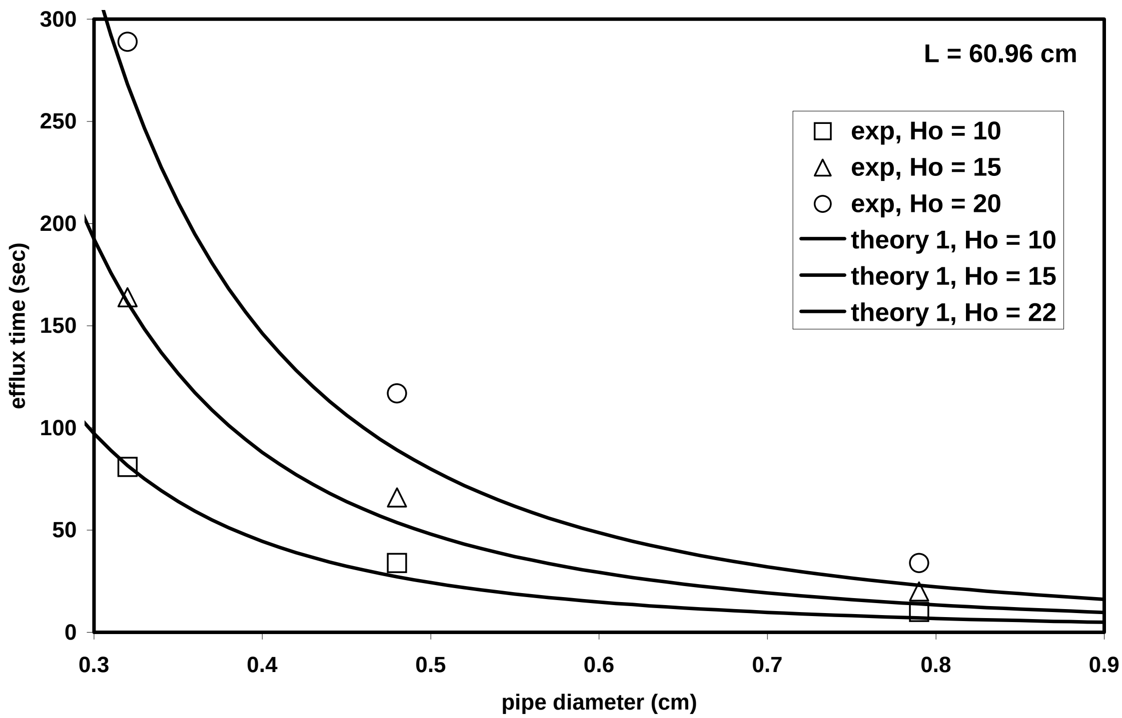

Figure Three. Efflux time as a function of pipe diameter, using the pipe of Length 60.96 cm and initial water heights of 10, 15, and 20 cm. The theory lines represent Case One, equation (8).

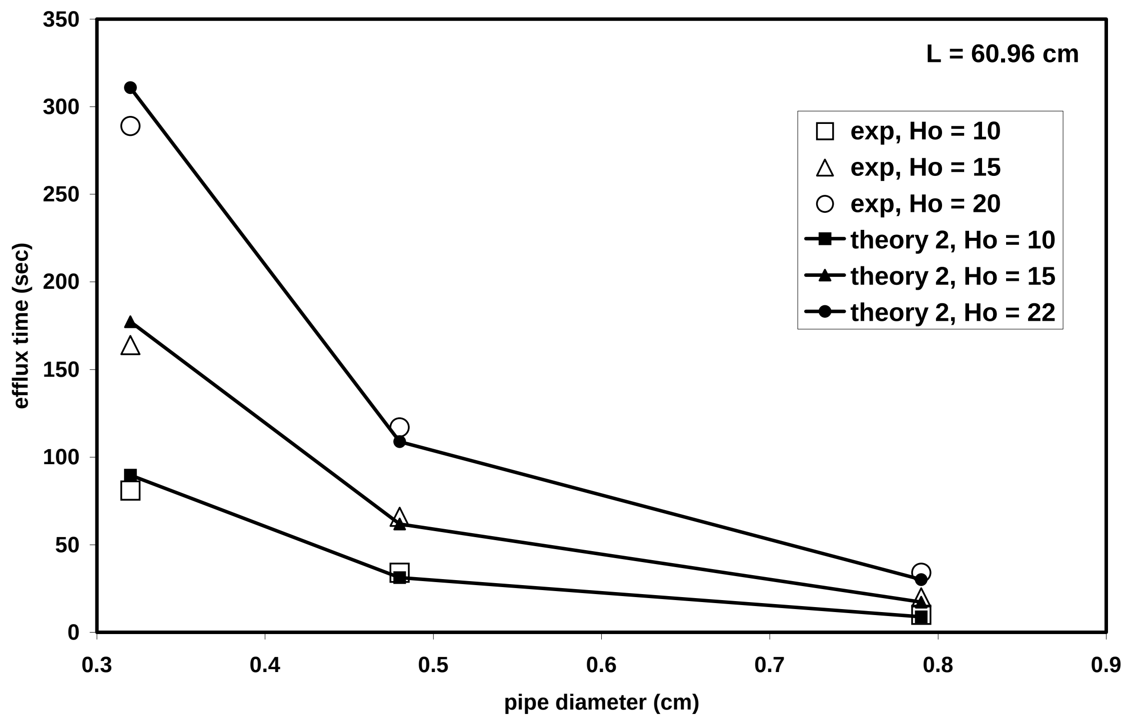

Figure Four. Efflux time as a function of pipe diameter, using the pipe of Length 60.96 cm and initial water heights of 10, 15, and 20 cm. The theory lines represent Case Two, equation (16).

Examination of Published Examples

Example 1. Theoretical Example

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

Here we briefly examine the 11 figures in this manuscript.

Figure 1. The purpose of this manuscript is to show that a particular procedure can reproduce an interaction potential. It is important because the intention is to use this procedure where the interaction potential is unknown. We first test it for a case where the interaction potential is known. This figure describes the validation procedure used in the manuscript.

Figure 2. This figure shows that in a three-body interaction between atoms 1, 2 and 3, the various combinations of stretching (S) and nonbonded (N) interactions that can exist in a diatomic system.

Figure 3. This figure shows a comparison of the PCF obtained from simulation and theory at two different densities. Note that the high density PCF is shifted 0.5 units up on the y-axis for better clarity. This kind of shifting must be noted in the caption. The simulation results have markers and the theory results have lines. The legend designates only the important distinction between the four data sets (theory vs simulation and high vs low density).

Figure 4. PCFs as a function of density. These are shifted by 0.25 units on the y-axis for visual clarity. The legend is replaced by labels near the curves.

Figure 5. Interaction energies as a function of density. These curves have also been shifted. Note that there is only one label for both simulation and theory results.

Figure 6. A comparison of a poor approximation (eq (1)) and the theory. Again, the curves are shifted. The explanation of the dashed and dotted lines is given in the caption. There is only one label for each pair of curves. One can visually observe that the agreement becomes worse as the density increases. We included this plot only because a reviewer of the manuscript asked that it be included.

Figure 7. The cavity function. Here we use arrows to identify each curve. A more traditional legend in a box could also have been used.

Figure 8. Here we show two PCFs (nonbonded and stretching) in the same plot. Combining plots in this way may not always be possible, but neither plot alone was interesting enough to warrant a separate figure.

Figure 9. A conventional comparison between simulation and theory. There is also an empirical fit to the simulation data, which overlaps the theory.

Figures 10 & 11. See notes for Figure 8 and 9 respectively. These figures are at high density.

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

Here we briefly examine the 7 figures in this manuscript.

Figure 1. The reactions relevant to this work.

Figure 2. Electron micrographs. One for each particle type, showing the differences in structure.

Figure 3. pH change. Note the line at zero to separate regimes. The data points are connected by straight lines.

Figure 4. adsorption amount vs time. Simple, large markers. Easy to see.

Figure 5. Adsorption amount vs pH. Again, simple clear markers.

Figure 6. Adsorption amount vs salt concentration. See Figure 5.

Figure 7. Schematics for the interactions in acidic, neutral and basic solutions.

Basic Rules for Formatting Tables

The basic formatting rule for tables is that they must be perfectly clear. There is no reason for a Table to have any confusion or ambiguity associated with it whatsoever.

Examination of Published Examples

Example 3.
[Liu *et al.*, *J. Phys. Chem. C* ***114****(25)* (2010)]

Here we briefly examine the 7 tables in this manuscript.

Table 1. Defines the system size.

Table 2. Defines the system density for the forty systems simulated. Note the organization of the headings to group columns in materials in order of increasing equivalent weight.

Table 3. Characteristic distances for some of the simulated systems.

Table 4. Accessible volumes and surface areas.

Tables 5-7. Mean distances and diffusion coefficients for water and hydronium ions. The same organization of headings that was used in Table 2 is used again here. The reader is already familiar with this organization, so keep it. Units are given in the caption.

References

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3. Kim, J.M., D.J. Keffer, B.J. Edwards, and C. Baig, *Visualization of Conformational Changes of Linear Alkanes & Short Polyethylenes under Shear and Elongational Flows.* J. Mol. Graph. Mod., **2008**. **26**(7): p. 1046-1056.
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