Technical Manuscript Writing for Doctoral Candidates

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Module 10. The Methods Section

I. Parts of the Methods Section

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

- describe the materials used
- describe synthesis and/or characterization procedures
- describe equipment used in the procedures
- describe numerical techniques used in modeling
- provide derivations used in a theoretical approach

Let us review the Methods 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)]

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)
- 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)

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

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)

We examine below how this structure of the methods section accomplishes the five tasks listed above.

I.A. Materials

Methods sections frequently include a description of the materials involved. Sometimes, the materials section is simply a list of chemical used. Sometimes, if the procedure involves a complicated nanostructured material, then there must be a more comprehensive characterization of the material. Let's be clear, if the paper is about using, for example, a known membrane to determine if it is successful at a given separation application, then the characterization of this membrane, including it pore size distribution, or crystallinity or whatever relevant property is of interest can be included in the materials section. However, if the manuscript is about synthesizing a new polymer membrane, this all of this characterization would go in the Results and Discussion section. In the materials section, you are only providing a description of the materials used in the experiment of interest.

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

The first paragraph in section 2.1. of this manuscript contains information regarding the materials used in the synthesis procedure of the nanoparticles. In this case, the description is limited to the names of the reagents and the commercial vendors.

I.B. Synthesis and/or Characterization Procedures

Descriptions of synthesis and characterization procedures belong in the methods section. If you are developing a new procedure, then you must provide a step-by-step detailed description. If you are simply using an established procedure, then a much shorter description with appropriate references to the original source should be included.

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

The two paragraphs in section 2.1. of this manuscript contain information regarding the synthesis procedure of these nanoparticles. The two paragraphs in section 2.2. of this manuscript contain information regarding the characterization procedure of these nanoparticles for Boron adsorption.

I.C. Equipment

Descriptions of important or unique equipment belong in the methods section. If the equipment is "stock" (unmodified) equipment available from a commercial vendor then the description can be quite brief, often times no more than a parenthetical remark after mention of the equipment.

If the equipment is a home-made vacuum chamber with custom designed sputtering nozzles and in situ XPS capabilities, etc. etc. etc. then a more complete description of the equipment may be appropriate with a photograph and/or schematic of the device.

Example 2. An Experimental Manuscript

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

The description of the equipment used in this work is spread through the relevant experimental procedures. Most of the descriptions appear as parenthetical remarks after mention of the equipment.

I.D. Simulation Methods

Like experimental techniques, computational techniques should be described in the methods section. Here, the amount of details included in the description is not always well established. Few journals will actually allow enough details to be presented that would make it possible for readers to reproduce the simulation results. Typically, you are limited to a few key points. Additional details on the methods, if necessary, can be included in the supporting information.

Example 1. A Theoretical Manuscript

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

In this manuscript, both paragraphs in Section II. Simulation describe the numerical procedures used in this work. These paragraphs contain a very brief but fairly complete description of the molecular dynamics simulations.

I.E. Theory

Theoretical Manuscripts can include derivations in the place where experimental papers have methods sections. The theory sections serve the same purpose as the methods section. They present the materials and procedures by which the theoretical apparatus is assembled and applied to the problem at hand.

As was mentioned in the module on equation, there are several important points to recall. It is expected that not every step in the derivation will be included. Instead, one may include some text describing the missing steps. For example, one might say, "Substitution of equation (2) into equation (4) and subsequent rearrangement for X yields" before providing the next equation. Make sure to include the important equations. Where possible, give physical explanations for each term in the equation. Lengthy derivations of previously published models should not be included. Derivations can be included in supplementary information or in an appendix. If inclusion of the derivation is very important, it should be included in the appendix, which will appear in the same pdf document as the article. If the derivation is included so that specialists may examine it if interested, it should appear in the supplementary information. Moving a derivation from the theory section to either the appendix or the supplementary information makes the paper more readable.

Example 1. A Theoretical Manuscript

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

In this manuscript, all six paragraphs in Section III. Theory describe the theory used in this work.