MONTANA TECH
Department of Metallurgical & Materials Engineering

EMET 5260
Thermodynamic Modeling of Aqueous Systems
Instructors: Dr. C.A. Young and Dr. H.H. Huang
Lecture: MWF 8-8:50a.m., ELC 204
Laboratory: Computer Homeworvs/Learning STABCAL
Office Hours, ELC 208A and ELC 215, Spring
12:00-1:00p.m. TR
or by appointment

2009-10 Catalog Description:
Reviews principles of thermodynamics appropriate for aqueous systems. The course then focuses on
obtaining and measuring thermodynamic data, making the information consistent with various data bases,
and using the data for modeling environmental, geochemical and metallurgical systems.

Credits: 3 Credit-Hours (3.0 Lecture)

Designation: Elective

Prerequisites: Senior or Graduate Standing and Consent of Instructor

Labs/Trips: Most Homeworvs and Demonstrations will involve Computer Usage

Textbook: Handouts will be distributed in class and/or made available on-line using Blackboard.

References:
   1965.
   Pergamon, 1966 (reprinted by NACE, 1974).

Relationship of Course to Metallurgical & Materials Engineering Program Outcomes: Course is
thermodynamic modeling course with emphasis on hydrometallurgy, waste water treatment, aqueous
chemistry, and geochemistry. Students will use thermodynamic information to model various water
systems at equilibrium based on free energy data that is available or can be determined from entropy and
enthalpy data. Students will also learn how to model titration, adsorption and non-equilibrium systems as
well. Introductory chemistry courses are essential as prerequisites. The course involves processing and
design and essentially helps to conclude the undergraduate program and/or begin the graduate program.

Objectives: The course introduces the student to thermodynamic modeling as well as the problems and
constraints of doing so properly.

Outcomes: Graduates of this course will or will be able to:
1. Understand that thermodynamic modeling is only as good as the data being used and that constraints
   must be appropriately identified and satisfied.
2. Understand that thermodynamic modeling is used for predicting equilibrium conditions but can be
   used on non-equilibrium systems as well.
3. Understand how models can be developed for special systems such as titrations, adsorption, etc.
4. Perform hand-calculations of simple systems and thereby gain an appreciation for computer models.
5. Use computer software, i.e., STABCAL, for the thermodynamic modeling of aqueous systems.
6. Be prepared for employment and success in industry as well as graduate school.
7. Meet **ABET Outcomes** a, k and o (consult the Course Catalog and Department Guidelines).

**Topics:**
Most topics are accompanied with homeworks:
1. Review of Thermodynamics (2 classes)
2. Databases and Consistent Data (3 classes)
3. High Temperature Data (2 classes) – Criss-Cobble and Helgeson et al.
4. Alpha Diagrams (2 classes)
5. Log Activity–pH Diagrams (2 classes)
6. Potential($E_H$)–pH Diagrams (3 classes)
7. Adsorption and Non-equilibrium Constraints (1 class)
8. Mass-balanced and Electron Density Constraints (1 class)
9. Computer Models (1 class)
10. STABCAL (6 classes)
11. Case Studies (7 classes) – examples include titrations, radicals, arsenic, corrosion, batteries

**Homeworks:**
At least 5 homeworks will be given along with 5 computer projects. The homeworks will typically be hand calculations and thereby will be a small portion of the computer projects. Reports are needed for each computer project and, like the homeworks, may involve outside reading and library searches. All are time-consuming and will help tie the lectures together.

**Projects:**
Most topics are illustrated through computer projects using STABCAL.

**Computer Use:**
Speciation and stability diagram calculations using STABCAL and associated thermodynamic databases.

**Attendance:**
 Attendance is critical and can lower the final grade by as much as two letters.

**Grading:**
The final grade will be weighted from course elements approximately as follows:

- Homeworks (45%)
- Laboratory Reports (20%)
- Computer Work (20%)
- Attendance (15%)

**Examinations:**
This course is heavy on homeworks and computer lab assignments and therefore does not have exams (unless attendance is poor).

**Professional Components:**
- Engineering Topics: 50%
- Design Component: Yes
- Computer Usage – Yes
- Ethics – No
- Statistics – No
- Safety – No

**ABET Outcomes Covered:** a, k and o (consult the Course Catalog and Department Guidelines)

**Prepared by:** C.A. Young ________
**Date:** October 22, 2009