Department of Chemical and Materials Engineering

CME 458 or 459 Special Project Course

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Each of 458 and 459 is a complete self-standing course,
and may be taken by either a Chemical or Materials student.
If a student takes it once, it is called "**CME 458**". The second time it will be called "**CME 459**".
Both courses cannot be taken in one term.

SYLLABUS Fall 2017/Winter 2018

as of August 8, 2017

Policy about course outlines can be found in Section 23.4(2) of the University Calendar.

Course description: individual research project under the supervision of an academic faculty member.

Credits: 3.5 (each)
The course starts:
September 5, 2017 (Fall Term; registration deadline with no academic record is September 18);
January 8, 2018 (Winter Term; registration deadline with no academic record is January 19).
The course ends (final report due): December 8, 2017 (Fall Term); April 13, 2018 (Winter Term).

Required weekly allocated time: to be discussed with the project supervisor; the recommended "in-class" time is at least 5 hr per week + 2-3 hr per week of "homework" time

Instructor and coordinator
The research project is performed under the supervision of an academic faculty member. The list of the CME Faculty members and their contact information can be found at:
http://www.cme.engineering.ualberta.ca/FacultyStaff/FacultyAcademicStaff.aspx

The course coordinator ensures student's registration, collects reports and assigns final grades (subject to the Dean's approval) based on recommendations from the supervisor.

Course coordinator: Dr. Natalia Semagina. Office: Donadeo ICE building, 12-330.
E-mail: semagina@ualberta.ca.

Important dates

Progress report deadline:	November 6, 2017, 4 pm (Fall Term); March 12, 2018, 4 pm (Winter Term)
Final report deadline:	December 8, 2017, 4 pm (Fall Term); April 13, 2018, 4 pm (Winter Term).

The reports' submission must be done both via e-mail of a pdf file to course coordinator semagina@ualberta.ca and a hard copy must be submitted to the Assignment box. If your report is too large to fit in, bring it to Project coordinator before the deadline time. It is student's responsibility to ensure that the report is received in time.

Late submission

10% of the final mark will be deducted if the progress report is not submitted on time. One each business day of delay to submit the Final report results in 10% mark deduction.

Note that the deadline extension is not possible, except for the reasons outlined at the University calendar (section 23.3 "Attendance", such as incapacitating illness, severe domestic affliction, or religious convictions).

Grading principles

This is not a pass/fail course. The course coordinator will assign the final grade based on the supervisor's recommendation and evaluation form, and will submit the grade to the Dean's office for approval.

100% mark is based on the Final Report evaluation form. The Evaluation form is completed by the project supervisor. The Final Report Evaluation raw score will be lowered by 10% for the failure to submit a progress report in time, and by 10% for each working day of delay of the Final report.

For the percentage of the report evaluation, refer to the Evaluation form (appendix). A student passes the course with a score of 3 out of 5 or higher (after all applied deductions). A necessary condition to pass the course, along with the total score of 3, is that at least the "satisfactory" mark is assigned in both "Intellectual contribution to the project" and "Analytic content: quality of treatment".

How to register

Note: a student cannot register on-line for this course. The registration form must be submitted to the Project coordinator for the registration.

1. The course is open only to Chemical or Materials students with a GPA of 3.0 or greater during the previous two academic terms. The prerequisite to CME 459 is CME 458.
2. Select a project from the Project List (Appendix), discuss it with a supervisor, complete the registration form (Appendix), obtain the signature from the Supervisor and e-mail the scanned form to the Project coordinator, who will complete your registration.
3. If a desired project is not included in the Project List, a student is encouraged to discuss such a project with the professor whom she/he considers best qualified as supervisor of the project. A brief written project description (title and one-page abstract) must be prepared and the project must be approved by the CME 458/459 coordinator (via e-mail). After that, the registration form should be signed and submitted as explained above.
4. A CME 458/459 project may not be combined with a Dean's Research Award as the Award "can't be concurrent with a project for which credit is received."

Requirements to the reports

1. The Progress Report should be 1-2 pages long, summarize the work done on the project and tasks still to be performed ("list" format is recommended). It is not graded per se, but the failure/delay of submitting it will result in 10% final mark deduction. Its purpose is to track student's progress. Start the report with your name, student ID, supervisor(s) name, project title and report date.
2. Final Report. There is no required page limit (unless indicated by the supervisor), please make sure that the content matches the evaluation criteria in the evaluation form (Appendix), unless a different report outline was approved by the supervisor and course coordinator. Typically, the report is about 20-30 pages (not including appendices with raw data, if any). The title page must contain your name, student ID, supervisor(s) name, course and project title and report date.

For the CME 459 project, please keep in mind that this is a separate report, not cumulative with your previous CME 458 report. If any data from the CME 458 report is used, they should be properly cited and distinguished from the current work.

All reports must be e-mailed as a pdf file and a paper copy must be submitted to the Assignment box before the deadline time. If your report is too large to fit in, bring it to Project coordinator before the deadline time. It is student's responsibility to ensure that the report is received in time. The course coordinator will distribute the reports to the appropriate supervisor(s). The late submission will be penalized as discussed above.

Academic integrity

The University of Alberta is committed to the highest standards of academic integrity and honesty. Students are expected to be familiar with these standards regarding academic honesty and to uphold the policies of the University in this respect. Students are particularly urged to familiarize themselves with the provisions of the Code of Student Behaviour (online at www.uofaweb.ualberta.ca/governance/studentappealsregulations.cfm) and avoid any behaviour which could potentially result in suspicions of cheating, plagiarism, misrepresentation of facts and/or participation in an offence. Academic dishonesty is a serious offence and can result in suspension or expulsion from the University.

Audio/video recording

Audio or video recording of lectures, labs, seminars or any other teaching environment by students is allowed only with the prior written consent of the instructor or as a part of an approved accommodation plan. Recorded material is to be used solely for personal study, and is not to be used or distributed for any other purpose without prior written consent from the instructor.

CME 458/459 Special Projects in Materials Engineering

DEPARTMENT OF CHEMICAL AND MATERIALS ENGINEERING

REGISTRATION FORM

Indicate which course you will be registering for:
*If a student takes it first time, it is called "**CME 458**". The second time it will be called "**CME 459**".*

CME458 _______ CME 459 ________

Term in which the project is to be completed (circle):

Fall Term (Sept-Dec) **Winter Term** (Jan-April) **Spr/Sum Term** (May-Aug)

Name of Student: ___________________________________ ID No. ________________

GPA in the last two full academic terms: ________
The course is open only to Chemical or Materials students with a GPA of 3.0 or greater during the previous two full academic terms

No. of Project in Listing: _______
If your Project is not listed, please provide a short written description of the project to the Course Coordinator

Title of Project: ____

Short Title of Project: ____
Mandatory. Must be maximum 55 characters including spaces and punctuation. This short title will appear in your official transcript

Supervisor(s): ____
(Full name)

Signature of Supervisor(s): ____

Signature of Course Coordinator: ____
Dr. Natalia Semagina

**** For CPC and Oilsands stream students only, approval is required from appropriate advisor.**

Please indicate program: Chemical CPC ________ Chemical Oilsands _________

Name: __________________________ Signature: ______________________________
(Please print) **(Advisor)**

DEPARTMENT OF CHEMICAL AND MATERIALS ENGINEERING

Final Report Evaluation Form

Project: CME 45___ Term:____________ Student_____________________________ID: _______________

Supervisor(s) *(Print name):* ____

Co-supervisors*: if the work was equally shared, each of you may provide your own evaluation and the coordinator will use the average value. Alternatively, upon agreement, you may submit one Evaluation Form signed by both of you.*

Evaluation criteria:

A student passes the course with a score of 3 out of 5 or higher (after all applied deductions) and only if at least the "satisfactory" mark is assigned in both "Intellectual contribution to the project" and "Analytic content: quality of treatment". The Final Report raw score will be lowered by 10% for the failure to submit a progress report in time, and by 10% for each working day of delay of the Final report. The course coordinator will assign the final mark based on the evaluation and supervisor's suggestion, and submit it to the Dean's office for approval.

Criteria:	**% of the mark**	**Excellent (5 pts)**	**Good (4 pts)**	**Satis-factory (3 pts)**	**Unsatis-factory (0 pts)**	**Max. score (max pts*%)**
Intellectual contribution to the project	25	☐	☐	☐	☐	1.25
Analytic content: quality of treatment	25	☐	☐	☐	☐	1.25
Overall command of the topic	10	☐	☐	☐	☐	0.5
Organization of content	4	☐	☐	☐	☐	0.2
Introduction: clarity of motivation and objectives	5	☐	☐	☐	☐	0.25
Thoroughness of the literature review, incl. state-of-the-art references	10	☐	☐	☐	☐	0.5
Conclusions and/or perspectives: informativeness and conciseness	5	☐	☐	☐	☐	0.25
Overall appearance	3	☐	☐	☐	☐	0.15
Grammar and spelling	4	☐	☐	☐	☐	0.2
Style (academic writing) and clarity	9	☐	☐	☐	☐	0.45
TOTAL	**100%**					**5 pts**

Other comments (if any): *The supervisor may suggest a grade. If more than one student is supervised, please indicate the approximate ranking, which the course coordinator will take into consideration*

Signature(s) of the supervisor(s), date ____

************************ **To be completed by the Course Coordinator** *********************

Final report handed in ☐ on time, ☐ with delay _____ days. Progress report handed in ☐ on time, ☐ not on time

Raw score based on the above evaluation:_______________ Final score after deductions:_______________

Final letter grade:___________________ Course coordinator:_________________________________

Natalia Semagina

CME 458-459 PROJECT LIST 2017-2018

The Project List includes only some representative projects. If a desired project is not included in the Project List, a student is encouraged to discuss such a project with the professor whom she/he considers best qualified as supervisor of the project. A brief written project description (title and one-paragraph abstract) must be prepared, and the project must be approved by the CME 458/459 coordinator.
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Project 1: Refractive index studies
Supervisor: Arno de Klerk
Type of project: Experimental
Number of students: 1

A challenge constantly faced by the oilsands industry, as well as by researchers conducting investigations related to oilsands bitumen conversion, is that of bitumen characterization. The bitumen and converted bitumen can usually not be analyzed by techniques that give compound specific information, such as gas chromatography. Bulk analysis techniques are employed instead. One bulk analysis technique that proved its value over many decades is refractive index. The measurement is straight forward and inexpensive to perform.

Considerable effort was put into refractive index measurement as petroleum refining developed, but the work was focused mainly on deriving compound class compositions in narrow cut naphtha and distillate range materials. The reason for this limitation is that refractive index is strongly affected by density. Within a narrow boiling range, there is not much variation in the density of species in each compound class. This makes the interpretation of refractive index difficult when there is inherently no control over the distillation range of the sample.

It is also difficult to measure the refractive index and density of very viscous and/or semi-solid materials. One way around this problem is to dissolve the material that has to be measured in an appropriate solvent and then measure the refractive index and density of the solution. Since the refractive index of the solvent on its own can be measured, one can in principle obtain the refractive index of the material on its own by calculation, if the binary mixing rule for refractive index is known. A number of binary mixing rules have been suggested in literature, but literature is not clear on which rule is best, or would be most appropriate for bitumen-solvent mixtures.

The objective of this work would be to experimentally evaluate binary mixing rules for refractive index and specifically to evaluate binary mixing rules for the refractive index of bitumen-solvent mixtures.

Project 2: Kinetic study of Athabasca vacuum residue in the presence of metal halides
Supervisor: Arno de Klerk and Glaucia Prado
Type of project: Theoretical
Number of students: 1

Different metal halides (NaCl, $MgCl_2$, $CaCl_2$) are naturally present in bitumen and their presence is not desirable in bitumen processing, since they cause fouling and corrosion of equipment. Nevertheless, it is known that some metal halides are catalyst for different types of reactions. It is then hypothesized that the presence of metal halides in oilsands upgrading cannot only affect physical processes, but can also influence the kinetic parameters of thermal cracking reaction. Therefore, this study aims in determine kinetic pyrolysis data of Athabasca vacuum residue in the presence and absence of different metal halides from thermal gravimetric analysis data. Thermal decomposition will be based on Arrhenius equation for calculation of pre-exponential factor and activation energy parameters.

Project 3: Correlation for liquid viscosity estimation
Supervisor: A. de Klerk
Type of Project: Theoretical
Number of Students: 1

One of the pure compound physical properties that are only poorly predicted by estimation procedures is liquid viscosity. Although there are many correlations available, as summarized in "Properties of gases and liquids" (many editions of this book), it is also clear that none of the correlations can be relied upon to always have good predictions, even for simple molecules. This can possibly be ascribed to the limited set of useful properties that can be employed for useful physical property correlations, but more likely it is because the true origin of viscosity is poorly understood.

The objective of this project is to determine what properties affect liquid viscosity most. For this purpose the intent is to make use of an extended range of pure compound properties to develop a correlation for pure compound liquid viscosity.

The work will be theoretical (computational) in nature. Guidance will be provided with respect to the type of properties that should be considered. The property values will be obtained from the literature using the Reaxys Beilstein-database. One suggested approach to the identification of the most relevant properties is the use of principal component analysis (PCA). Another suggested approach is to make use of hierarchical clustering. Training and assistance will be provided for the application of both methods.

Project 4: Novel hydrogel materials for skin-adhesive biosensors
Supervisor: Hyun-Joong Chung
Type of Project: Experimental

Most tissues in biological systems are soft, whereas conventional electronic devices are made of hard materials. When the electronic devices can be flexible/stretchable with a good adhesion to human skin, the resulting device can be easily wearable to monitor physiological parameters from human body. Imagine band-aid or Tegaderm to monitor human health! Hydrogel is the key material to realize the grand goal of my research program. A specific target for the student project is (i) to study the fundamental physical chemistry of the hydrogel materials and/or (ii) to develop hydrogel materials for energy devices, wound dressings, or other practical applications.

Project 5: Blood glucose sensor
Supervisor: Stevan Dubljevic
Type of Project: Computational
Term: Winter 2018

The fast and reliable glucose sensor needs to be realized as simple input-output relationship between the changes in the blood glucose concentration and sensing device, see Fig.1. In particular, we are looking in the representation in the following form:

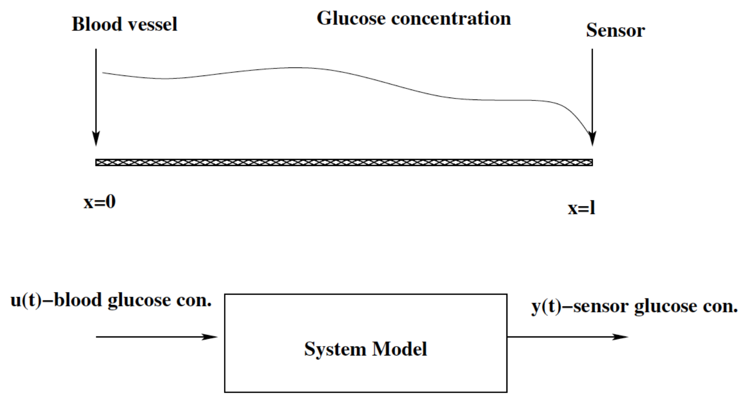

Figure 1: The schematics of glucose concentration profile from the blood vessel to the sensor.

The important aspect of the model is that sensor data are discrete functions in time, that is a measurement of the glucose that is registered at sensing cite, which is taken in some time intervals. In other words, the output of the model is discrete function of time y(t) → y(k) where **k** -represents time instance. Having the spatially distributed nature of the system on one side, the discrete measurements of glucose taken at the time sample instances which are specified by the sensor features on the other, one needs to incorporate all these aspects in robust, cheap, and reliable sensing mechanism to address accurate enough on-line real measurement of glucose in blood.

Project 6: Solidification of an aluminum bulk metallic glass
Supervisor: H. Henein
Type of Project: Experimental

Bulk metallic glasses are a new class of materials characterized by their amorphous structure under low cooling rates of solidification. The resultant alloy has high hardness and low ductility. Some of these new classes of alloys are incorporated into new designs of golf clubs. A new Al based bulk amorphous alloy will be atomized and the structure characterized using x-ray, and microscopy techniques. The hardness of the alloy will also be measured. A model of droplet cooling will be used to estimate the droplet cooling rate prior to solidification. The resultant structure and properties will be related to the droplet cooling rate.

Engineering objectives:
•Develop experimental testing strategy.
•Carry out atomization experiments.
•Use of various microscopy techniques to characterize the solidified microstructure.
•Carry out x-ray diffraction analysis of powders.
•Use hardness measurements to estimate the mechanical properties.
•Relate mechanical properties to the evolution of microstructure.

Project 7: The Effect of Warm Rolling on the Morphology of Cementite in Low alloy Steels
Supervisor: H. Henein
Type of Project: Experimental

Low alloy steels are used for down hole applications in the oil and gas sector. As down hole conditions of oil and natural gas extraction are worsening, producers encounter the presence of hydrogen sulfide with consequences such as sulfide stress cracking (SSC) instigated by hydrogen. There is increasing evidence that the morphology of cementite in these quench and tempered steels plays a role in the SSC behaviour. The objective of this project is to explore the use of warm rolling as a processing strategy to modify the morphology of cementite. The project will involve carrying out a literature review on the subject, plan and execute an experimental warm rolling test matrix, followed by the quantitative characterization of the microstructure using Optical and SEM microscopy, X-ray diffraction. In addition, other characterization techniques such as hardness measurements may be used as needed. An analysis of the experimental and characterization results will be carried out.

Project 8: Additive Manufacturing of Polymers, Metals and Composites
Supervisor: H. Henein (hani.henein@ualberta.ca)
Type of Project: Experimental
Number of students: up to 3 (including projects 5 and 6). Preference will be given to students doing both CME 458 and 459 (in consecutive terms).

The approach of Additive Manufacturing (AM) presents many opportunities to revolutionize manufacturing. There are today numerous approaches to carrying out AM. There is, however, a paucity of data and knowledge about the properties of the materials being processed. The level of porosity, the microstructural evolution, the surface finish, the mechanical properties are amongst the issues of interest. There are several projects available to generate knowledge on these aspects of several AM processing approaches.

Project 9: Development of Novel Bifunctional Catalysts for Rechargeable Zn-air Batteries
Supervisor: D.G. Ivey (780-492-2957 and doug.ivey@ualberta.ca)
Type of Project: Experimental
Number of Students: 1 per project

Peak oil and the effects of global warming have encouraged the development of new alternative energy storage devices such as supercapacitors, fuel cells and batteries. Zinc-air batteries are a promising candidate because of their high energy density, cost-effectiveness and environmentally-friendly nature. Rechargeable Zn-air batteries have potential applications in various areas such as portable electronic devices and electric vehicles. In a Zn-air battery, the oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) occur at the air electrode (cathode) during charge and discharge, respectively. Currently, the overall performance and lifetime of zinc-air batteries is limited by the lack of effective bifunctional electrocatalysts for ORR and OER at relatively low overpotential. Although Pt and Ir based catalysts exhibit the best overall bifunctional activity, their high cost and limited availability necessitate the fabrication of new non-precious metal catalysts.

Several potential catalysts materials are been investigated, including transition metal oxides and intermetallics. The work will involve fabricating, characterizing and testing candidate materials using methods such as electrodeposition, x-ray diffraction, electron microscopy, cyclic voltammetry and rotating disk electrode analysis.