

## ChE352A: Chemical Process Simulation Lab (1-0-2-5)

**Lecturer:** Professor Vishal Agarwal  
**Office:** Room 466, Faculty Building  
**Email:** vagarwal@iitk.ac.in

**Lectures:** Wednesday 2pm-2:50pm, L10  
**Labs:** Thursday (Group 1) 2pm-3:50pm, CC-01 Windows Lab  
 Friday (Group 2) 2pm-3:50pm, CC-01 Windows Lab

**Office Hours:** Monday 2-3pm or by appointment

**Assessment:** 10% for class participation/quizzes, 30% for assignments, 30% for mid-sem, 30% for end-sem. **Zero-tolerance policy on academic dishonesty**

**Assignments:** Reading assignments, Lab assignments, and Home assignments.  
 Assignments will not be accepted after due date and time. **NO MAKE-UP FOR LAB**

**Examination:** 3hrs, in computational lab. One make-up exam at the end of the semester for those who missed the end/mid-sem with a valid reason.

**Course Contents.** Approximate number of lectures/labs for each topic are given below. I might make slight modifications as the course progresses. We will use Matlab as well as process simulation package such as ASPEN.

Topic	Lectures + Labs
<b>Introduction to process modeling and simulation</b>	$\frac{1}{2}$
<b>Ideal and non-ideal VLE (Txy-Pxy plots, Azeotrope):</b> Computation of VLE data (Temperature-composition, Pressure-composition plots) using (i) ideal mixture assumption and (ii) using various activity coefficient models such as Wilson, Van-Laar model, UNIFAC etc. Special emphasis on VLE of azeotropic mixtures.	$1\frac{1}{2} + 2$
<b>Flash distillation and continuous binary distillation with reflux:</b> Composition of vapor and liquid streams in a flash distillation still using VLE data. Material balance/enthalpy balance in the plate columns. Computation of ideal number of plates using optimal reflux ratio.	2 + 2
<b>Multicomponent distillation with reboiler and condenser:</b>	1 + 1
<b>Mass transfer between gas and liquid:</b> Study of absorption, reaction and diffusion processes in a contact reactor/bubble absorber/packed tower/plate column through a two film model.	1 + 1
<b>Heat exchange equipments:</b> Design and optimization of single effect and multiple effect evaporator. Design of a shell and tube heat exchanger	2 + 2
<b>Reactor-separator problem:</b> In the first lab, complete material and energy balance for a given reactor-separator system will be carried out. The choice of correct specification variables (recycle ratio, product purity, yield etc) for convergence of material balance/energy balance. In the second lab, optimization of the process will be carried out.	2 + 2
<b>Real case studies:</b> In these labs, students will study the utility of process simulators in real industrial scale processes. Examples include: (i) simulation of cumene production process, (ii) Ammonia synthesis, (iii) manufacture of vinyl chloride monomer and hydrodealkylation.	2 + 2
<b>Laminar flow:</b> through a circular pipe (solution by hand calculations, as well as by simulator), generation of grid, flow visualization, simulation of developing flow in a pipe (if time permits).	2 + 2
<b>Total</b>	14 + 14

**Teaching Assistants:** Prakash Tiwari (tprakash@iitk.ac.in)  
Nachiket Vivek Kuntla (nvkuntla@iitk.ac.in)  
Amit Kumar Sahu (amitsk@iitk.ac.in)  
Jaishri Jain (jainj@iitk.ac.in)  
Nikhil Srivastava (nikhilsr@iitk.ac.in)  
Piyush Kumar Singh (piyushs@iitk.ac.in)

### Suggested References

There is no text book for this course. The course material will be taken from several sources. Some of the useful references are given below.

1. Finlayson, Bruce A. Introduction to chemical engineering computing. John Wiley & Sons, 2012.
2. Jana, Amiya K. Chemical process modelling and computer simulation. PHI Learning Pvt. Ltd. 2011.
3. Luyben, William L. "Heuristic design of reaction/separation processes." *Industrial & Engineering Chemistry Research* 49 (2010): 11564-11571.
4. Luyben, William L. "Design and control of the cumene process." *Industrial & Engineering Chemistry Research* 49 (2009): 719-734.
5. Green, Don W., and Robert H. Perry. "Perry's Chemical Engineers' Handbook." (2008).

In addition, standard chemical engineering books on thermodynamics, mass transfer, fluid mechanics, chemical reaction engineering may be used.

### Some Points to Keep in Mind.

1. **Learning is your responsibility.** It is my responsibility to teach but it your responsibility to learn. Pay utmost attention during lectures, and keep up with the reading materials. Don't be shy, ask questions during lectures or after lectures. Please remember engaging is the best way to learn.
2. **Homework Problems.** First try working the homework problems independently. If you have difficulty moving forward even after several tries, please ask for help either from me during office hours or from TA's or from your peers. I encourage you to discuss homework problems in groups but when you sit down to finally write your homework, it should be done independently; and it should reflect your understanding of the problem.
3. **Grade is Just a Number.** Don't get into the race of just getting grades. Your aim should be to learn, understand, and master the subject. This requires a painful struggle through lectures, texts, and homeworks. Everyone has different backgrounds and has different speeds of learning; so invest the required time. Remember that: "Rome was not built in a day".
4. **Think Critically and Challenge Yourself.** Critical thinking is possibly one of the most important skill that will help you in whatever you do in life. This course is an opportunity to develop that habit. Think critically about what you read and about homework problems. Don't be satisfied by just solving problems or understanding course contents. Challenge yourself to go beyond the class lectures and homework problems.

## Academic Dishonesty.

Please read the following carefully (taken from <https://www.winona.edu/business/96.asp>):

1. **Cheating:** Using or attempting to use unauthorized materials in any academic exercise or having someone else do work for you. Examples of cheating include looking at another student's paper during a test, bringing a crib sheet to a test, obtaining a copy of a test prior to the test date or submitting homework borrowed from another student.
2. **Deception and Misrepresentation:** Lying about or misrepresenting your work, academic records, or credentials. Examples of deception and misrepresentation include forging signatures, falsifying application credentials and misrepresenting group participation.
3. **Enabling Academic Dishonesty:** Helping someone else to commit an act of academic dishonesty. This would include giving someone else an academic assignment with the intent of allowing that person to copy it or allowing someone else to cheat from your test paper.
4. **Fabrication:** Refers to inventing or falsifying information. Examples of fabrication include drylabbing (inventing data) or making references to sources you did not use in academic assignments.
5. **Plagiarism:** Using the words or ideas of another writer without proper acknowledgement, so that they seem as if they are your own. Plagiarism includes behaviour such as copying someone else's work word for word, rewriting someone else's work with only minor word changes and/or summarizing someone else's work without acknowledging the source.

## Pledge

I, do solemnly promise that

1. I will maintain the highest standards of academic honesty during this course.
2. I have carefully read above forms of academic dishonesty and I will not indulge in any of them. If I am caught indulging in any one of them, I deserve one and only one grade, i.e., F.
3. I will maintain at least 90% of attendance in this course.
4. I will not be late for this class.

*"Try not be a man of SUCCESS but rather try to become a man of VALUE" — Albert Einstein*