

THERMODYNAMICS, KINETICS, AND CHEMICAL FUNDAMENTALS

- ✓ 1. For a series reaction, what variables influence the amount of intermediates formed? How would you maximize the production of intermediates in a CSTR, a PFR, or in a batch reactor?
- ✓ 2. For an exothermic, first order reaction, plot the extent of reaction and the reaction rate as functions of temperature.
- ✓ 3. When can the steady-state approximation be used?
- ✓ 4. What is the chemical potential?
5. Experimentally how would you determine ΔH_f , ΔG_f , ΔS_f ?
- ✓ 6. How does a refrigerator work? Sketch T-S, P-V and/or P-H diagrams.
- ✓ 7. How does the rate constant vary with temperature?
- ✓ 8. Derive design equations for mass and energy for CSTR, PFR and batch reactors.
- ✓ 9. Define space time, space velocity and mean residence time.
- ✓ 10. What are the Clapeyron and Clausius-Clapeyron equations?
11. How would you calculate the adiabatic flame temperature?
- ✓ 12. Which type of reactor is best for a series reaction? a parallel reaction? an autocatalytic reaction?
- ✓ 13. Give the three laws of thermodynamics.
14. Diagram the Carnot cycle, the Otto cycle, the diesel cycle, the Brayton cycle and the Rankine cycle.
- ✓ 15. Derive a Langmuir-Hinshelwood expression for a solid catalyzed reaction, e.g. $A+B \rightarrow R$
- ✓ 16. Prove that $\Delta G \leq 0$ for any process.
- ✓ 17. Prove that S tends towards a maximum.
- ✓ 18. What is the Gibbs mixture rule? Derive the Gibbs-Duhem relation.
- ✓ 19. For the reaction $A \rightarrow B \rightarrow C$, in which the activation energy for the second step is greater than that for the first, how would you adjust the temperature to maximize the production of B?
20. How do you calculate the equilibrium constant at non-standard temperature and pressure?
- ✓ 21. Define U, H, S, G, F, and A.
22. What is a Joule-Thompson liquefaction process?
- ✓ 23. What is the slope of an $\ln K_{eq}$ vs. $1/T$ curve for an exothermic reaction? an endothermic reaction?

- ✓ 24. If $\Delta G = 0$ at equilibrium, why isn't $\Delta G_{\text{rxn}} = 0$ for any reaction?
- ✓ 25. Give a physical interpretation of the activation energy.
- ✓ 26. Where does the Langmuir isotherm come from?
- ✓ 27. Why is entropy zero at 0 K?
7. 28. How would you calculate the total volume when two equal volumes of different liquids are mixed?
29. How would you calculate from first principles the heat capacity of two gases, e.g. H_2 and CH_3NCO .
30. Analyze a complete problem, from determining the chemistry of the important reaction step, to calculating the equilibrium conversion, transient response of the concentration and temperature and its ultimate effect on a macroscopic variable in the system, such as pressure in a closed vessel.
- ✓ 31. Sketch H/S , T/S , $\ln(P/H)$, P/T , and P/V diagrams for a pure substance.
- ✓ 32. What does polytropic mean?
- ✓ 33. How is the concept of reaction coordinate used?
34. What is the phase rule when reactions are occurring?
35. How does absorption refrigeration work? What are suitable characteristics of a working fluid?
36. Give three methods of liquefying gases.
37. Why is it necessary to use differential reactors for kinetics studies?
38. What is the difference between extent of reaction and equilibrium conversion?
39. Why is freon used in fridges instead of water, air, etc?
40. What is the activity and why is it different from fugacity?
41. What is fugacity and how is it calculated?
42. Consider Langmuir-Hinshelwood kinetics: why might the rate go down as the gas concentration goes up?
43. What would be the difference between activation energies determined in the regions where internal and external mass transfer dominate?
44. Why is the 3rd law important?
45. What does the temperature distribution in PFR look like? *see at 244*
46. What is a fluidized bed reactor and what are its advantages and disadvantages? *244 notes*
47. Find the enthalpy change for a pipe system consisting of a pump, a heat exchanger, and a vertical step of height h in series.

48. How do you find K_{eq} for $A + B = C$? *folded*
49. How do you get the rate constant from plug flow experimental data for a first order reaction?
50. For ideal gases what is ΔV_{mix} , ΔH_{mix} , ΔS_{mix} , and ΔG_{mix} ? How do we express these quantities for ideal solutions?
51. What is Raoult's Law? Henry's law? Where do they apply?
52. Can a Raoult's law solution have an azeotrope?
53. What is the Lewis fugacity rule? What is Amagat's law?
54. What is the difference between a mixing rule and a combining rule?
55. What is a maximum boiling azeotrope? Does it exhibit positive or negative deviations from Raoult's law? If a solution of this type is distilled will the azeotrope be recovered in the distillate or the bottoms?
56. What is the effect of adding an inert gas on the equilibrium between N_2 , H_2 , and NH_3 ?
57. Derive Maxwell's relations.
58. Which liquid phase equation of state allow for azeotropy? Phase separations?
59. What is the corresponding states theorem? What is its significance?
60. Describe the graphical approach to reactor design and analysis.
61. Derive an expression for the Joule-Thompson coefficient. What is the importance of its sign?
62. Derive the Michaelis-Menten rate equation.
63. What is a Thiele parameter? What is its usefulness?
- ~~64.~~ For the series reaction $A \rightarrow B \rightarrow C$ where the rate of the second reaction is much greater than that of the first, how would you maximize the selectivity of B over C?
65. Give the Van der Waals equation. What is the significance of the constants a and b? How would you estimate them given critical temperature and pressure data? What does the P-V diagram of a vdW gas look like? Where is the "correct" and where is it "wrong"? Where are the stable, unstable, and metastable regions?
66. Given a closed drum of organic liquid which reacts exothermically with traces of water present in the drum, derive all the equations necessary to describe the temperature and pressure in the drum as a function of time.

ΔH from calorimetric measurement