

Due: Workshop

Physical Chemistry II

Exercises Set 5

1. Conceptual

- What are the distinctive characteristics of the different forms of energy, potential energy, kinetic energy, and thermal energy?
- How is heat energy generated and transmitted by conduction and convection, as compared to radiative transfer?
- What are criteria for assessing combinations of probabilities for separate event types.
- What types of data are needed in application of Bayes' Theorem? What are its advantages?

2. Cellular Automaton Propagation Rules

For the one-dimensional ($d=1$) cellular automata considered in class which had $k=2$ possible states (0 and 1), the laws of propagation in time depended on the status of the cells in the immediate neighborhood domain (radius $R=1$) and the previous status of the cell itself. The entirety of possible rules turned out to be $N_R=256$.

- Write down an equation for N_R in terms of domain size, dimension of the CA, and the multiplicity k of states for each cell.
- How many propagation rules are possible for a CA in 3D, where each cell in 3-dimensional space can attain any of the 7 colors of the rainbow?

3. Heat Loss by Radiation



A solid red-hot iron ball of radius $R = 10$ cm is placed in a room of dimensions $5\text{m} \times 4\text{m} \times 3.5\text{m}$. It is exposed to the ambient air (18°C), cooling down from its original temperature of $T = 1273\text{K}$ by radiating heat energy Q according to the Stefan-Boltzmann Law (assume emissivity $\varepsilon = 1$, neglect the effect of the ambient temperature).

- a) Write down the differential equation for the cooling rate, dQ/dt .
- b) What is the temperature of the iron ball after $t = 1\text{hr}$?
- c) How long does it take for the ball to cool down to 25°C ?
- d) What is the final room temperature?

Data: The density of iron is $\rho = 2.7\text{g/cm}^3$, the specific heat of iron is $C_v = 0.451\text{ J/g }^\circ\text{C}$.

The density of air is $\rho = 1.2\text{g/L}$, its specific heat at constant volume is $C_v = 0.718\text{ kJ/kg}^\circ\text{C}$.

4. Probabilities for Combined Events

Consider a game using the outcome of rolling two perfect dice A and B . Calculate the probabilities for the following events:

- a) $P(A \wedge B)$ for $[A] = 6$ and $[B] = 6$
- b) $P(A \vee B)$ for $[A] = 6$ or $[B] = 6$
- c) $P(A \oplus B)$ for either $[A] = 6$ or $[B] = 6$, but excluding $[A] = [B] = 6$
- d) $P(\neg A \wedge \neg B)$ for neither $[A] = 6$ nor $[B] = 6$

5. Permutations

Take the sequence of different integer numbers $S_4 = \{1, 2, 3, 4\}$.

- a) Write down all cyclic permutations $P_c(S_4)$ of this set. Is there any difference between cw and ccw permutations?
- b) From the set of cyclic permutations constructed in a), generate all non-cyclic permutations $P_{nc}(S_4)$.
- c) What is the number of all different permutations of the set S_4 ?

- d) By complete induction, prove that the number of all permutations of a set of N objects equals $P_c(S_N) = N!$
- e) Assume that, in a set S_N of N integer numbers, m numbers are equal. What is the number of different permutations $P'(S_N)$?

6. Conditional Probabilities (AC)

A drug test is mandatory for airline pilots. A general estimate is that perhaps a small 5% of them may actually be users. The available drug test has been shown to be highly effective: It will indicate with 95% probability a true positive result for actual drug users, and will produce a true negative result for non-drug users in 97% of the cases. For the following assume a sample of $N=1000$ pilots are tested for the specific drug use. Start with your definition of the two events E1 and E2.

- a) How many of these persons are expected to be non-users?
- b) How many false positive test results can be expected from this group?
- c) How many true positive tests can be expected from this group?
- d) One person in the group tests positive. What is the likelihood of that person being an actual user of drugs? Apply Bayes' Theorem.