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Simulation to Measure Vapor Pressure with Different Temperatures

A working version of my simulation has been published on my website at:
http://sites.google.com/site/carollundssimulationsite/

My goal in creating this simulation is to expand on an example of an equilibrium system I currently use to bridge the topic of rates of reaction and equilibrium. I use the phase change of water because it is a system students have a familiarity with and an intuitive understanding of. I also use it because it points out many of the common misconceptions students have about equilibrium systems (including that concentrations are equal, heat of reaction is equal forward and reverse, rate constants are equal, etc) Most students know from reading the text that equilibrium is defined as equal rates forward and reverse but many do not understand what the equilibrium constant represents or how concentrations of reactants and products can be different and the system can be at equilibrium. The water system offers many good examples and explanations for these misconceptions.

I have used standard conditions (25C, 1.0L, d=1.0g/ml) as my preliminary states for the system and occasionally used another temperature (such as 80C) to compare the difference in vapor pressure at a higher temperature but only in passing. I did not realize the extent of the information available from this system until preparing the simulation and seeing the graphs of the different conditions along side each other. The value of presenting many experiments together is enormous in enabling students (and teachers) to see connections between properties.

This simulation allows students to experiment with a closed system of liquid water and water vapor at various temperatures and enables students to collect and analyze data concerning the temperature, pressure, and concentration (molarity) of the phases of water in the system. The goals of the simulation are to provide students with a model for understanding the properties of an equilibrium system, the effect of temperature on the rate of a reaction, on the position of an equilibrium system, the calculations required to convert between pressure and moles for a gas, the conversion between Kp and Kc for an equilibrium system in which gases are present at a range of temperatures.

The Topics Covered by this Simulation include:
1. Equilibrium Vapor Pressure of a Liquid in a Closed System at a range of temperatures.
2. Rate of Evaporation of water at different temperatures.
3. Concepts of an equilibrium system:
    a) What is equal at equilibrium?
    b) What may not be equal at equilibrium?
    c) What is "constant" at equilibrium?
    d) How do values for Kp and Kc compare?
    e) Kevaporation and kcondensation
4. Comparison of molarity of water at different temperatures.

5. Comparison of density of water at different temperatures.
6. Good example of use of the Clausius–Clapeyron equation to find the enthalpy of vaporization.
7. Application of vapor pressure graph to phase diagram for water.

Some additional benefits of the simulation include enhanced development of students' problem solving skills by requiring the analysis of larger quantities of data than students normally generate in the laboratory and making comparisons between graphed data for several trials at one time. Students will also be required to use the ideal gas law to calculate moles and molarity of water vapor from partial pressure data, use changing molarity of liquid water to understand the "constant" nature of pure liquids and pure solids in equilibrium systems, and the determination of equilibrium concentrations/pressures to calculate Kc and Kp. Students will be able to see first hand the effect of temperature on values for Kc and Kp, and be able to plot pressure vs. temperature to estimate a value for the enthalpy of vaporization.

Experimentally the simulation is a valuable tool because it replicates data that is difficult to determine and quickly provides values for equilibrium vapor pressures at wide range of temperatures. The actual experiments require a considerable amount of time and equipment (constant temperature water baths, pressure sensors, computer interface to measure timed changes in pressure). The simulation provides data at a range of conditions not easily measured in lab, provides the ability to change parameters easily, and allows students to compare multiple sets of data quickly.

The science of the simulation includes the relationship between vapor pressure and temperature for a water equilibrium system. I calculated the molarity of water at different temperatures using the density of water at each temperature. I experimentally measured the rate of evaporation at two different temperatures to get an approximation of the time required to reach equilibrium in the specific conditions of the simulation.

To calculate a vapor pressure at a given temperature I used the following equation:

$$P = 6.112* e^{(17.62T/243.12 + T)}$$

 (http://cires.colorado.edu/~voemel/vp.html)

In the above equation, temperature is in Celsius and pressure is in hPa's. I wanted the pressure values to be in kPa's so I adapted the equation in the simulation to be: $P = (6.112 *e ^{(17.62T/243.12 + T)})/10$

Values for density and vapor pressure of water can be found at: http://en.wikipedia.org/wiki/Properties_of_water#cite_note-6

I checked the equation to confirm that it produced vapor pressures that matched published values and I also graphed lnP vs. 1/T(inK) and found a value for the enthalpy of vaporization

that matched published values. I have included tables of my calculated values and published tabulated values for a comparison

My calculated values using the above equation:

Temp C	Temp (K)	Pressure (kPa)
0	273	0.6112
5	278	0.872
10	283	1.226
20	293	2.333
25	298	3.160
30	303	4.234
40	313	7.367
60	333	19.993

The published values found at:
http://en.wikipedia.org/wiki/Properties_of_water#cite_note-6

Temperature		Pressure[18]	
°C	K	Pa	atm
0	273	611	0.00603
5	278	872	0.00861
10	283	1,228	0.01212
12	285	1,403	0.01385
14	287	1,599	0.01578
16	289	1,817	0.01793
17	290	1,937	0.01912
18	291	2,064	0.02037
19	292	2,197	0.02168
20	293	2,338	0.02307
21	294	2,486	0.02453
22	295	2,644	0.02609
23	296	2,809	0.02772
24	297	2,984	0.02945
25	298	3,168	0.03127

The vapor pressures and temperatures give a good approximation of the enthalpy of vaporization (43.424 kJ/mole), which compares to published enthalpy values at the range of temperatures used in the simulation.

Temperature (°C)	Heat of vaporization H_v (kJ mol^{-1})[7]
0	45.054
25	43.99
40	43.35
60	42.482
80	41.585
100	40.657
120	39.684

From http://en.wikipedia.org/wiki/Properties_of_water#cite_note-6

To approximate rate data for the simulation, I measured the time (in a 1 liter container) to reach equilibrium (approximately 70 to 80 seconds) and using the change in molarity (calculated from the vapor pressure and temperature), I approximated the rate of the reaction based on the time it took to reach equilibrium and the number of moles of water vapor that formed.
For k condensation I used the following approximations:
ln2/11 sec at 10°C
ln2/10 sec at 20°C
ln 2/9 sec at 30°C
ln2/8 sec at 40°C
ln2/7 sec at 50°C
ln2/6 sec at 60°C

I then used kevaporation and the molarity of water vapor at equilibrium to approximate kcondensation using the molarity of water liquid at equilibrium. To calculate the molarity of water initially present I used temperature and density of water and 1.0L total volume. To find molarity at equilibrium I used molarity initially present minus molarity (moles of water vapor formed).

Temp °C	Temp (K)	Pressure (kPa)	Molarity of H_2O vapor at equilibrium	Initial Molarity of H_2O liquid	Equilibrium Molarity of H_2O liquid	kevap	kcond
0	273	0.6112	2.692841E-4	55.49977	55.4995	2.8020E-7	0.05775
10	283	1.226	5.21067534E-4	55.49217	55.49164893	5.9157E-7	0.063
20	293	2.333	9.577168E-4	55.40916	55.40820228	1.197833-6	0.0693

25	298	3.168	1.2787E-3	55.34481	55.3435313	1.6843E-6	0.0729
30	303	4.234	1.680731E-3	55.26823	55.266549	2.341675E-6	0.0770
40	313	7.367	2.831E-3	55.07571	55.072879	4.4528E-6	0.086625
60	333	19.993	7.221E-3	54.57614	54.5689	1.5284E-5	0.1155

I used density of water at each temperature from the link below and a molecular weight of water of 18.0152 g/mol to find molarity. http://www.newton.dep.anl.gov/askasci/chem03/chem03872.htm

1. What the simulation does:
    a. Generates "experimental" data for the vapor pressure of water in a closed system at four different temperatures (20°C, 30°C, 40°C, and 60°C).
    b. Generates "experimental" data for the initial and equilibrium concentration (molarity, "M") of liquid water at four different temperatures (20°C, 30°C, 40°C, and 60°C).
    c. Generates data for change in concentration (M) of liquid water and change in vapor pressure of water vs. time at four constant temperatures (20°C, 30°C, 40°C, and 60°C).
    d. Students are able to graphically enter Temperature values in C and generate a corresponding vapor pressure for a range of Temperatures from 0°C to 100°C.
    e. Allows students to analyze graphs for pressure vs. time to compare reaction rate and equilibrium positions
    f. Allows students to construct a pressure temperature graph from the equilibrium positions in the pressure time data
    g. Students can use the pressure values to calculate Kp for water at various temperatures
    h. Students can compare the molarity of pure water at different temperatures to calculate density of water at different temperatures and to observe that molarity and density of water change with temperature
    i. Students can construct a density temperature graph for water
    j. Students can use Pressure and Temperature data to create a graph of lnP vs. 1/T (K) and find average value for ΔHvap of water (data gives value of 43.424 kJ/mole) Students will need to convert Temperature in Celsius to Kelvin and recognize that slope of graph = −ΔH/R, so need to multiply slope by R to get ΔH in Joules then convert to kJ to compare to tabulated value.

What the simulation does not do:
    a. The rate data is intended to be merely representative of the time difference for each temperature but does not represent the actual values for the rate or rate constant for the evaporation process. Assuming you measure the rate of evaporation from a pure

sample of liquid water at a constant temperature, the evaporation rate depends primarily on the surface area of the liquid water in the container, a property that can vary widely given the procedural method described, and the composition of the air above the surface of the liquid. The amount of water vapor present in the air above the liquid will affect the rate of evaporation and the ultimate amount of water that evaporates.