Worksheet: Determine Antoine constants for saturation pressure

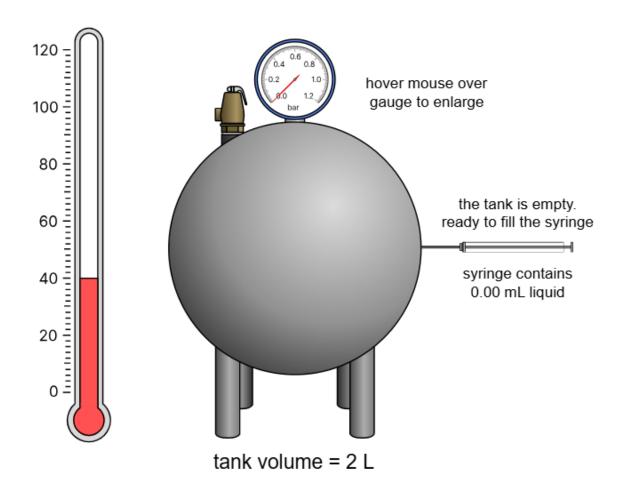
Name(s)______

This experiment measures the saturation pressure (vapor pressure) of a single component over a range of temperatures by injecting sufficient liquid into an evacuated tank at constant temperature to obtain vapor-liquid equilibrium. The constants in the Antoine equation are determined from a series of temperature/pressure measurements. The heat of vaporization is obtained from the Clausius-Clapeyron equation.

Student learning objectives

- 1. Be able to describe how saturation pressure changes with temperature.
- 2. Be aware of how saturation pressure can be measured.
- 3. Know how to fit data to a model to determine parameters.

Equipment



- A spherical tank in a constant-temperature bath. The tank has a port through which a syringe
 injects liquid. The pressure gauge on the tank reads absolute pressure. The maximum
 operating pressure of the tank is greater than the saturation pressure of the liquids at high
 temperatures, and a pressure relief valve prevents pressures above the tank rating.
- A vacuum pump (represented by the reset button) evacuates the tank.
- A heater and temperature controller (represented by a temperature slider) adjust the temperature of the tank.
- A beaker of liquid (not shown) and a liquid syringe.

Questions to answer before starting the experiment

This experiment measures saturation pressures by injecting liquid into an evacuated tank. Would more or less liquid need to be injected at higher temperatures to determine saturation pressure? Why?

Suppose sufficient liquid were injected at 50°C to measure saturation pressure. What happens if more liquid is injected?

Given a limited temperature range for experiments because of the pressure rating of the tank, and given that you want to obtain the heat of vaporization from the Clausius-Clapeyron equation:

$$\ln(P^{\text{sat}}) = -\frac{\Delta H_{vap}}{R} \frac{1}{T} + I$$

where the temperatures are absolute temperatures (K), how should the temperatures chosen for measurements be distributed in the range? That is, should the temperatures be equally spaced in the temperature range or in the inverse temperature range? Explain why.

Before starting

Evacuate the tank (with the reset button) so that the pressure gauge reads zero absolute pressure.

Select a molecule (A, B, C, D, E) to inject from the dropdown menu. Note that the Antoine constants are only good over a temperature range, as indicated by the range of the temperature slider.

Molecule selected	
Temperature range	

Measure saturation pressures.

Select the amount of liquid to inject: _____ mL.

Pick the first temperature to make measurements.

Inject liquid with the syringe, allow the tank to equilibrate, and read pressure from the pressure gauge. How can you determine if you are at vapor-liquid equilibrium (VLE)?

Either inject more liquid or change the temperature (keeping in mind how the measurements should be spaced in the temperature range) and repeat measurements until sufficient data are obtained to yield accurate Antoine constants. Ensure that the system is in vapor-liquid equilibrium at each temperature. Record the data in the table below.

Temperature (°C)	Pressure (bar)

Determine Antoine constants.

The Antoine equation is:

$$log P^{sat} = A - \frac{B}{T + C}$$

Note that this log is base 10.

Although Excel Solver can determine the Antoine parameters, it may have difficulty obtaining the best fit. Another approach is to use the LINEST function in Excel to apply multivariable linear

regression to fit the saturation pressure (P^{sat} , bar) versus temperature (T, °C) data in the table to a linearized form of the Antoine equation.

$$\log P^{sat} = A + (AC - B)\left(\frac{1}{T}\right) + (-C)\frac{\log P^{sat}}{T}$$

In this equation, the two independent variables (from your measurements) are $\left(\frac{1}{T}\right)$ and $\frac{\log P^{sat}}{T}$ and the dependent variable is $\log P^{sat}$ on the left side of the equation. This is calculated from the right side of the equation.

Values of the Antoine parameters (A, B, C) with their units obtained from a multivariable linear regression:

A = _____

B = _____

C = _____

Plot In P^{sat} versus inverse <u>absolute temperature</u> and use the Clausius-Clapeyron equation to estimate the heat of vaporization (ΔH_{van} , kJ/mol) of the molecule.

$$ln(P^{sat}) = -\frac{\Delta H_{vap}}{R} \frac{1}{T} + I$$

where R is the ideal gas constant, P^{sat} is the saturation pressure at temperature T, and I is a constant.

$$\Delta H_{vap} = ____ +/- ___$$

Questions to answer

- 1. Are the measurements valid if the tank is at high pressure (or low temperature) so that the gas phase is not ideal? Explain.
- 2. What are sources of error in the measurements?
- 3. Using literature data and your measurements of the heat of vaporization and the Antoine constants, which of these molecules is most likely your molecule? benzene, toluene, methanol, ethanol, n-octane, n-heptane, water, iso-octane, cyclohexane
- 4. What safety measures would you employ if making this measurement in the laboratory?