

FYS2160, lab2: Phase transitions,

In this project you will study the gas–liquid phase equilibrium of the van der Waals fluid. You will compare the heat of vaporisation of the van der Waals fluid to that of water and to Trouton’s rule. To do so you will use both analytical and numerical methods. You will also do MD simulations of ice, water and water vapour and discuss the order, entropy and latent heats in relation to the experiments and Trouton’s rule.

Document your work and what you learn and deliver one single, coherent ”report” with the following requirements

- include both experiments, analytical and numerical work in the same report
- the report should have the following parts
 - ”Introduction”
 - Main body. This includes (methods,) results and discussion, but you may subdivide the text in any way you find best.
 - ”Summary” or ”Conclusions”
- there should be a red thread through the report connecting the different parts. This should be established in the Introduction. The results should be discussed in relation to the red thread and in the end you should summarise the relations between the different parts of the study and how they relate to the red thread.
- the report and all figures and labels should be easily readable.
- do not copy text, lists of equipment and units and procedures and method descriptions from the lab texts.
- do include your observations of events and difficulties during your experimental and numerical work.
- the report should be delivered at the end of the day.
- the report should be a single PDF file.
- Do *not* include code listings in the report. If you want to submit code, it should be uploaded as a separate .py file.

You have to formulate your own red thread, but in this Lab the keywords are *latent heat*, *Trouton’s rule*, *water*, *microscopic structure*, *order and entropy*.

I. NUMERICAL PART: PHASE COEXISTENCE BY MD AND IN THE VAN DER WAALS EQUATION OF STATE

A. Molecular dynamics of ice, water and vapour

In this subproject you will perform MD simulations in Lammmps to get a feel for the structure and dynamics of the three phases of water, ice 1h (the common form of ice we all know), liquid water and water vapour. Do the simulation, study the output and include your observations in the report. Try to include both direct observations and what you can infer about entropy and latent heat.

1. About the simulations

One key part of this lab, is that you will not run multiple independent Lammmps-simulations. Instead, the end of each simulation you run will be used as the starting point for the next. The first simulation you will run is that of ice. After this, you will run a simulation to melt the ice. Before evaporating the ice, you will first have to run a short simulation to expand the simulation cell, before you finally melt the ice.

2. Simulation details

We have borrowed starting configuration and thermalization procedures from O'Brien [4]. Go the web page and download the three files `water.in`, `forcefield.SPCE` and `restart.250K`. The first file is the input file for running the Lammmps simulations. The second is a file determining the interaction between atoms in the simulations. This is read by the input file. The third file is a restart file, which contains the state of the atoms at the end of a simulation that has was run at 250 K. This file is also read by the input file and used as the starting point for the first simulation you will run.

First you will run an ice simulation. Depending on your computer, the simulation will take between 5 and 10 minutes.

- Put the input files `water.in`, `forcefield.SPCE` and `restart.250K` in your simulation directory.
- Make a copy of the input file, naming it `water_251K.in`. You will now edit `water_251K.in` to run 10 000 timesteps at 251 K, dumping the trajectory information every 10th timestep.
- Line 2: `variable T equal 251`
- Line 39: `run 10000`
- Run the simulation: `lmp -in water_251K.in`.

While waiting for the simulation to end, we will try to understand what the input file does. In line 7, `restart.250K` is read, and used as the starting point

of our simulation. In line 26, we choose to run the simulation at a fixed volume, temperature and number of particles. That is, the temperature of the box is held at 251 K throughout the simulation making the ice increase its temperature by 1 K. The dump file created should be named `water_251K.lampstrj`. This is automatically ensured by the temperature variable `$T`. Once the simulation is done, you should have a file named `restart.251K`, which is specified in line 40.

- Change the name of the log-file `log.lammps` to `log_water_251K.lammps` to prevent it being overwritten.
- Do *not* change the name of the `.lampstrj` file, as the new dump files we create will get a different name automatically when we run the next simulations at different temperatures.
- Open the trajectory file in Ovito to visualise the simulation. Discuss and comment.

Now you will melt the ice, starting from the end of our previous simulation. We will double the steps of this simulation, to 20 000 timesteps, so the simulation will take between 15 and 25 minutes to complete.

- Make a copy of the input file `water_251K.in`, naming the new file `water_300K.in`.
- Line 2: `variable T equal 300` (choosing a temperature above the melting point).
- Line 7: `read_restart restart.251K`
- Since ice and water have different densities you have to run the simulation in the (NPT) ensemble instead of the (NVT) ensemble to allow the volume change:
 - Comment out the `nvt` line (line 26).
 - Uncomment the `npt` line (Line 28).
- Line39: `run 20000`
- Run the simulation: `lmp -in water_300K.in`.
- Once the simulation is done, change the name of the log-file `log.lammps` to `log_water_300K.lammps`.
- Plot the energies (E_{tot} and H) dumped in `log_water_300K.lammps` and discuss.
- Open the trajectory file in Ovito to visualise the simulation. Can you observe some of the structures mentioned in the appendices in the experiment lab text? Discuss and comment.

Because it is unlikely to get vapour nucleation in the tiny liquid volume you must first expand the simulation cell. When looking at the previous simulations in Ovito you probably noticed that the particles are quite clustered, with little free space to move around. To expand the box, you will run a short simulation at 301 K, thereby preventing file overwriting.

- Make a copy of the input file `water_300K.in`, naming the new file `water_301K.in`.
- Line 2: `variable T equal 301` (Only increasing the temperature to prevent file overwriting).
- Line 7: `read_restart restart.300K`
- Line 23: Uncomment the line `fix 2 all ...`
- Line 26: Uncomment the `nvt` line.
- Line 28: Comment out the `npt` line.
- Line 39: `run 2000`.
- After the simulation is done, change the name of the log-file `log.lammps` to `log_water_301K.lammps`.
- Visualise the simulation in Ovito. Discuss and comment.

Now, we want to evaporate the water. However, this takes very long time. On my computer it took roughly 1.5 hours with 5 000 timesteps. Therefore, you will use log-file from the course web page to study the energy changes from this simulation.

- Download this file, named `log400K.in`.
- Plot the energies (E_{tot} and H) from this simulation, visualise and discuss.

If you have time at the end of the lab, you may run the evaporation simulation yourself. First, you should complete the tasks in section IB, where you will study phase transitions of a Van der Waals system.

To run the evaporation simulation, the procedure is as follows:

- Make a copy of the input file `water_301K.in`, naming it `water_400K.in`.
- Line 2: `variable T equal 400`
- Line 7: `read_restart restart.301K`
- Line 23: Comment out the line `fix 2 all ...`
- Line 26: Comment out the `nvt` line.
- Line 28: Uncomment the `npt` line.

For the number of steps, you may choose to run 5 000. Since this will take quite some time, you can run e.g. 1 000 steps at 400 K, then 1 000 steps at 401 K, then 1 000 steps at 402 K and so on. Make sure to rename the input files and log-files accordingly. If you plot E_{tot} and H after each simulation you will see whether the system has reached equilibrium.

- Line 39: `run *000`
- `lmp -in water_400K.in`
- Visualise the result in Ovito and discuss.

3. Two phases in MD

Calculating properties of the phase coexistence in MD is difficult in the very small systems accessible to us (a few thousand molecules can be simulated on a laptop in a reasonable time). One reason is that such a tiny two-phase system will be dominated by the gas-liquid interface and another reason is that nucleation of gas bubbles in water is completely dependent on the details of the boundary conditions [2]. To calculate accurate coexistence properties by MD one has to resort to theoretically advanced tricks [3].

B. van der Waals equation of state

The van der Waals fluid is a mean field theory of a gas. It is a model system, just as the ideal gas, although it includes more features of realistic gases. The van der Waals gas includes two of the main effects of an attractive two-particle interaction between particles in the gas: a repulsive interaction that keeps particles apart, and an attractive long-range interaction that pulls particles together. These two effects leads to two changes in the Helmholtz free energy of the gas, as compared to an ideal gas: Instead of the volume V we introduce the effective volume, $V - Nb$, where the volume b is the excluded volume per particle, and we introduce an average binding energy, $-a(N/V)^2$. Helmholtz free energy for the van der Waals fluid is:

$$F = -NkT \left(\ln \left(\frac{n_Q \cdot (V - Nb)}{N} \right) + 1 \right) - \frac{aN^2}{V}, \quad (1)$$

where $n_Q(T) = (2\pi mkT/h^2)^{3/2}$ is a function of T only.

In this lab you are to find if the van der Waals fluid liquid – gas phase transition follows the Trouton rule $\frac{H_v}{NkT_b} \approx 11$, where H_v is the heat (enthalpy) of vapourisation and T_b is the boiling temperature. In order to do this you will need to do some analytical work and some numerical work.

1. Analytical work

You will start with some analytical calculations. From the Helmholtz free energy of the van der Waals fluid, calculate analytically

$$\text{the pressure: } P = - \left(\frac{\partial F}{\partial V} \right)_{T,N},$$

$$\text{Gibbs free energy: } G = F + PV.$$

Use the critical parameters

$$P_c = \frac{a}{27b^2}, \quad V_c = 3Nb, \quad kT_c = \frac{8a}{27b},$$

to express the reduced parameters

$$\hat{V} = V/V_c, \quad \hat{T} = T/T_c, \quad \hat{P} = P/P_c,$$

and the dimensionless Gibbs free energy per particle

$$\hat{G} = \frac{8G}{3NkT_c} = -\frac{8}{3}\hat{T} \ln(3\hat{V} - 1) - \frac{3}{\hat{V}} + \hat{P}\hat{V} + f(\hat{T}),$$

where $f(\hat{T})$ depends only on \hat{T} and not on \hat{P} or \hat{V} . You can therefore neglect this part in the next steps where you will study how \hat{G} varies with \hat{P} and \hat{V} . See section 9.5.3 of the compendium.

2. Numerical work

Now you will do a numerical estimation of the latent heat of a Van der Waals system during a phase transition from a liquid to a gaseous state. By finding the boiling point pressure, $P(T_b)$, and the resulting volume change of the system, ΔV , you will use the Clausius-Clapeyron relation to compute the latent heat

$$\frac{dP}{dT} = \frac{\Delta S}{\Delta V} = \frac{L}{T\Delta V},$$

where $L = T\Delta S$ is the latent heat. At the boiling point, the change in Gibbs free energy is zero, so we have $\Delta G = \Delta H - T\Delta S = 0$. Thus, the latent heat, L , is equal to the enthalpy of vaporisation, H_v .

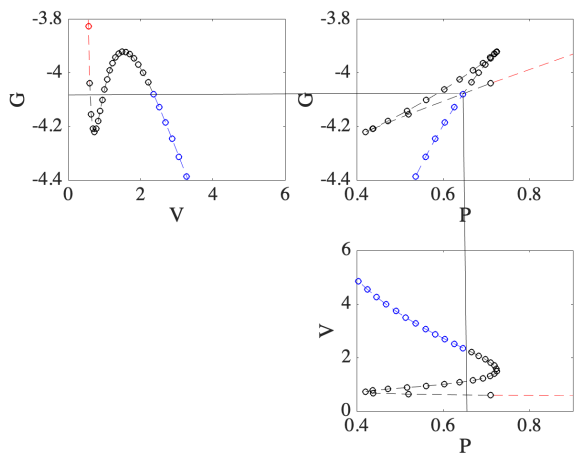


FIG. 1: Plots of reduced Gibbs free energy at $\hat{T} = 0.9$ and pressure for the same reduced volumes. The red part of the curve corresponds to the liquid phase, the blue part is the gas phase and the black part is the unstable part of the curve corresponding to the liquid-vapour coexistence. The black lines demonstrate how the equal area construction to find the coexistence pressure $\hat{P}_b(\hat{T}_b)$ corresponds to the self intersection of the $\hat{G}(\hat{P})$ curve.

We will only use dimensional quantities for the remainder of this task. Hence, you should use your analytical

expressions for $\hat{P}(\hat{V})$ and $\hat{G}(\hat{V})$, and the reduced parameters \hat{V} and \hat{T} . In Figure 1, the phase transition occurs at the self-intersection of the $\hat{G}(\hat{P})$ curve. The pressure at which $G_l = G_g$ corresponds to a change in volume $\Delta\hat{V}$, as seen in the bottom panel.

- Choose values of \hat{T}_b between 0.3 and 1. For each one, plot $\hat{P}(\hat{V})$, $\hat{G}(\hat{V})$ and $\hat{G}(\hat{P})$. Make sure your array of \hat{V} values has a suitable range, such that the self-intersection point is included. See Figure 1 for what you can expect.
- Determine the coexistence line numerically. For each value of \hat{T}_b , determine the coexistence pressure $\hat{P}_b(\hat{T}_b)$ by finding the pressure where $G_l = G_g$. Do this by eye, as the intersection point is difficult to determine numerically. Remember to plot the actual data points, and not just continuous lines. Write down the values of \hat{P}_b , and the corresponding volume change $\Delta\hat{V}$.
- Plot the coexistence line $\hat{P}_b(\hat{T}_b)$ for the values of \hat{T}_b you have used.
- Comment on the accuracy of your determination of the coexistence line.
- Use the Clausius-Clapeyron relation to determine the latent heat (heat of vaporization) H_v numerically for the van der Waals fluid. For the pressure derivative, you can try a simple finite difference approximation.
- It is found that for simple liquids the ratio $H_v/(RT_b) \sim 10$ between the enthalpy of vaporisation, H_v and the normal boiling point temperature, T_b . Over a much larger range of noble gases, organic and inorganic liquids and metals one finds $H_v/(RT_b) \sim 12$. This has been named Trouton's rule. Calculate \hat{H}_v/\hat{T}_b for the van der Waals fluid and plot it versus \hat{T}_b .
- Use the principle of corresponding states to map the van der Waals fluid to water that has critical temperature $T_c=647.096$ K and pressure $P_c=22.064$ MPa. Which \hat{T} and \hat{P} does "normal" pressure and temperature correspond to?
- It has been argued that Trouton's rule follows from the principle of corresponding states. Do you agree?
- Can you find an alternative explanation for Trouton's rule using the entropy change during vaporisation?

II. EXPERIMENTAL PART: MELTING AND VAPORIZATION

The goals of this lab exercise are for you to 1) understand the principles of calorimetry, 2) get training in lab-work, 3) relate measurement data to theoretical concepts, 4) acquire a deeper understanding of the nature of phase transitions and 5) learn about important properties of water.

Concretely, you are to measure the latent heat of melting and the heat of vaporization for water with uncertainties. We then want you to consult Trouton's rule and see if water follows this simple relation.

A. Introduction

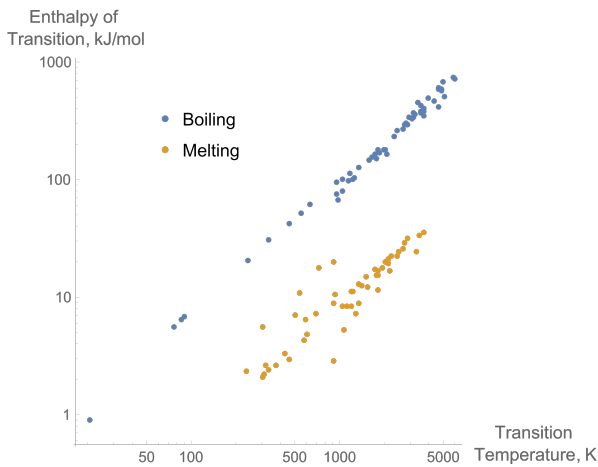


FIG. 2: Trouton's rule: Enthalpy of vaporization, H_v , and normal boiling point temperature, T_b , are proportional. Image from [7].

Measurements of heats of formation, melting and vaporization are necessary for calculation of many thermodynamic properties and to understand many processes in Nature, daily life and industry. Heats of melting and vaporization also display a certain regularity (see Figure 2) that is due to the change in order and entropy from one phase to another.

For the case of vapourization Trouton's rule may be stated as: $\frac{H_v}{RT_b} = \frac{\Delta S_v}{R} = 11 \pm 1$, where H_v is the enthalpy of vapourization, R the gas constant, T_b the boiling temperature and ΔS_v the entropy change on vaporization. In this exercise we will measure H_v , compare to Trouton's rule and try to understand the result.

For the case of melting the trend in Figure 2 is less convincing. There are still many materials that follow the linear relationship $\frac{H_m}{RT_m} = \frac{\Delta S_m}{R} = \text{constant}$, but there are more "outliers". In this exercise we will try to understand the reasons for this spread around the linear relationship and why water behaves as it does.

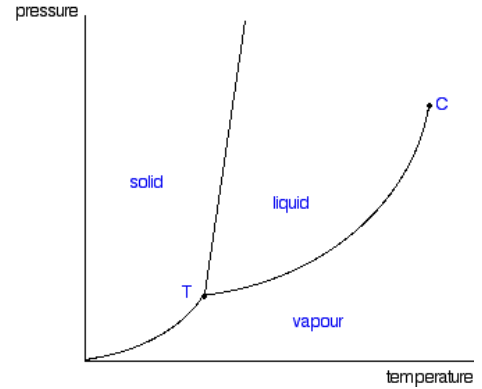


FIG. 3: Generic pressure-temperature phase diagram. Note that the solid-liquid coexistence line is much steeper than the liquid-gas coexistence line.

B. Calorimetry

Calorimetry is the process of measuring the amount of heat released or absorbed during a phase transition or a chemical reaction. The heat measurement is performed either at constant pressure or at constant volume. However, it is not possible to measure heat directly, we have to measure other quantities like temperature, pressure and electrical current and potential to derive heat capacities and heat. Both heat of melting and heat of vapourization can in principle be measured in two different ways:

1. by measuring the temperature and the amount of electric energy (Joule heating) added to melt/vapourize a known quantity of ice/water.
2. by exploiting the Clausius-Clapeyron relation

$$\frac{dP}{dT} = \frac{H}{T\Delta V} \quad (2)$$

and measure the slope of the pressure-temperature coexistence line.

1. Heat of melting

Since the solid-liquid phase coexistence line is very steep (see Figure 3) and solids and liquids are very incompressible it is impractical, not accurate or impossible to measure the heat of melting by using the Clausius-Clapeyron relation. Therefore we will use a calorimeter based on the principle shown in Figure 4 A. If we know the heat capacity C_0 of the calorimeter we can measure the heat absorbed Q_m to melt a known mass m of ice by measuring the temperature change inside the calorimeter. From the current I and the electrical potential U we know the rate of Joule heat, $dQ_{el}/dt = UI$ released in the water. The heat capacity C_0 is then measured without ice in the calorimeter from the relation

$$C_0 dT/dt = dQ_{el}/dt = UI. \quad (3)$$

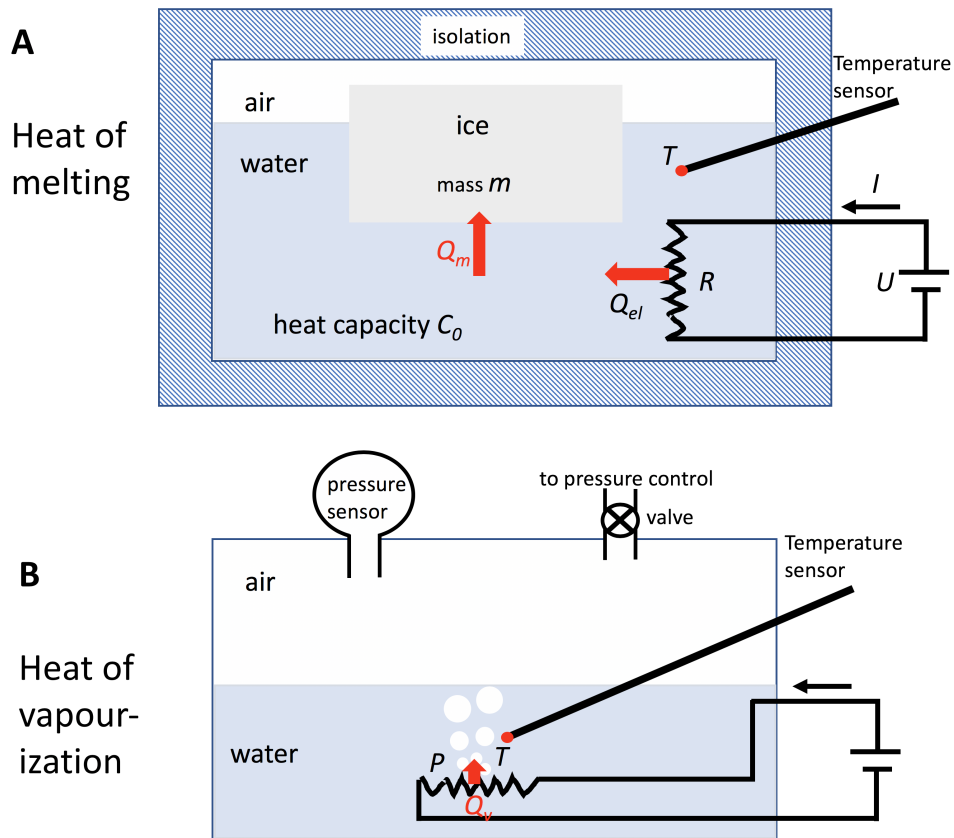


FIG. 4: Principles of measurement of heat of melting and heat of vapourization.

2. Heat of vapourization

According to the Clausius-Clapeyron relation (2) we only need to measure the pressure P and temperature T of some part of the coexistence line and know the volume change ΔV of the phase transition. This means one has to vary the pressure systematically in a practical range and measure the corresponding change in temperature necessary for the water to boil. The $\Delta V(T)$ of the phase transition of one mole of water we can calculate assuming that the vapour phase is an ideal gas:

$$\Delta V(T) = \frac{RT}{P} \quad (4)$$

C. Experimental

1. Heat of vapourization

We will measure the pressure as function of temperature, $P(T)$ of a water-vapour system where we assume 1) the two phases are in equilibrium, 2) the molar volume of water is negligible compared to the molar volume of vapour, 3) the vapour is an ideal gas and 4) the enthalpy (latent heat) of vapourization is constant in a

small temperature interval. The Clausius-Clapeyron relation 2 may then be reformulated as:

$$\ln \frac{P_1}{P_2} = -\frac{H_v}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right), \quad (5)$$

where $P_1(T_1)$ and $P_2(T_2)$ are two points on the liquid-vapour coexistence line.

- Close both valves and start the water aspirator pump.
- Open valve H_1 slowly and keep it open until the pressure reaches $2 \cdot 10^4$ Pa.
- Close the valve and shut off the water jet in the pump.
- Turn on the water cooling and heat the water to boiling.
- Regulate the heater to avoid violent boiling.
- When the water is still boiling and the pressure and temperature meters show fairly constant values the system is in a stationary state and the values $P(T)$ should be noted using the data logger.
- Estimate the accuracy of the measurements from the readings.

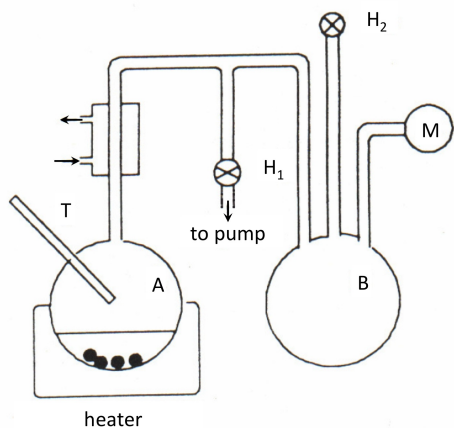


FIG. 5: Equipment for measurement of the temperature dependence of the vapour pressure. The flask A contains water and pebbles to avoid explosive boiling. A glass tube and a rubber tube connect the flask to the buffer volume B that makes the response of the system “softer”. Using the water aspirator pump the pressure inside the flasks can be reduced below the atmospheric pressure (about 10^5 Pa) to about $2 \cdot 10^4$ Pa. The pressure in the system can be controlled using the valves H_1 and H_2 . The glass tube connected to flask A can be cooled by cold water to condense the vapour into water that will drip back into the flask.

- Open valve H_2 carefully to increase the pressure by about 5 kPa.
- Repeat the measurement cycle until atmospheric pressure is reached.
- Plot $\ln P$ versus $1/T$ and do a least squares fit to determine H_v .
- Estimate the accuracy of the measured H_v from the experimental curve and the fit.

2. Heat of melting

The specific (molar) heat of melting for ice is the energy needed to melt 1 kg (1 mol) of ice at 0°C to water at $T_0 = 0^\circ\text{C}$. The calorimeter is a stainless steel container with a plastic lid surrounded by insulating material. A heating element and a stirrer is mounted on the plastic lid and a thermometer can be introduced into the calorimeter through a hole in the lid.

- Fill the calorimeter with about 1.25 l water at room temperature.
- Start the data logger (see appendix).
- Start the stirrer.
- Turn on the current in the heater and set it to 0.75 A.

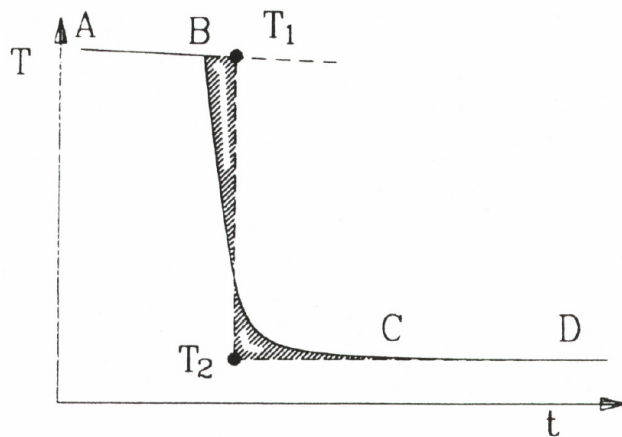


FIG. 6: Temperature evolution in the calorimeter during melting of ice.

- When the temperature reaches 30°C turn off the current to the heater.
- Compute the heat capacity C_0 of the calorimeter from the logged temperature and the Joule heating: $C_0 dT/dt = UI$
- Keep logging the temperature while stirring for at least 5 minutes while preparing to measure the heat of melting.
- Fetch an ice cube of about 250 ml from a water bath at 0°C .
- Weigh the ice cube without delay and put it into the calorimeter. Note the mass of the ice cube, m .
- Keep logging the temperature until it stabilizes for at least 5 minutes.
- Determine the temperatures T_1 and T_2 and enthalpy of melting H_m (see Figure 6 and text below).
- Estimate the accuracy of H_m that you found.

Figure 6 shows the typical temperature evolution during your experiment. The enthalpy (or latent heat) H_m of melting and the heating of the melted water to the surrounding temperature is supplied from the cooling of the calorimeter:

$$m[H_m + C_v(T_2 - T_0)] = C_0(T_1 - T_2), \quad (6)$$

where $C_v = 4200 \text{ J}/(\text{kg}\cdot\text{K})$ is the specific heat capacity of water at 10°C . The temperatures T_1 and T_2 are determined from the temperature log as in the diagram 6.

D. Questions

1. Compare the heat of vapourization H_v with Trouton's rule. Can you determine if the deviation is

due to inaccurate measurements or due to a particular physical phenomena?

2. The vapour phase in the bottle is a mixture of air and water molecules. Clearly the partial pressure P_w of water vapour is lower than the total gas pressure $P_{tot} = P_w + P_{air}$. Does this affect the measurements?
3. How would the measurements be affected if we turned off the water cooling? (The water cooling is there to make the water vapour condense)
4. Why do we measure the temperature in the gas phase and not in the water phase?
5. Why is the enthalpy of vaporisation much higher than the enthalpy of melting?

Appendix A: Radial structure of solids, liquids and gases

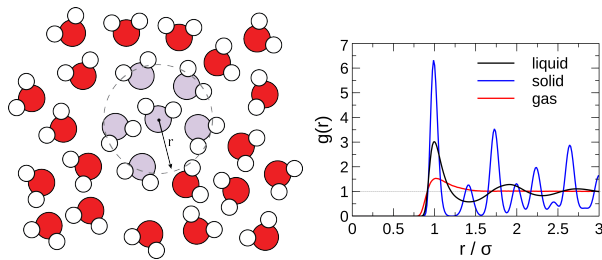


FIG. 7: The radial distribution functions (RDF). **Left:** The RDF defines the probability of finding a particle at distance r from another tagged particle. Here, the distance r is between the oxygen atoms of two water molecules. **Right:** The radial distribution functions of solid ($T = 50$ K), liquid ($T = 80$ K), and gaseous argon ($T = 300$ K). The radii are given in reduced units of the molecular diameter ($\sigma = 0.3822$ nm). Images from [6].

The radial distribution functions (RDF) characterises the radial structure around an atom or a molecule, but averages out all orientational order. The RDF shown in Figure 7 are typical for the three phases of matter, they do not change greatly from material to material (although chemists spend a lot of time interpreting the small differences...).

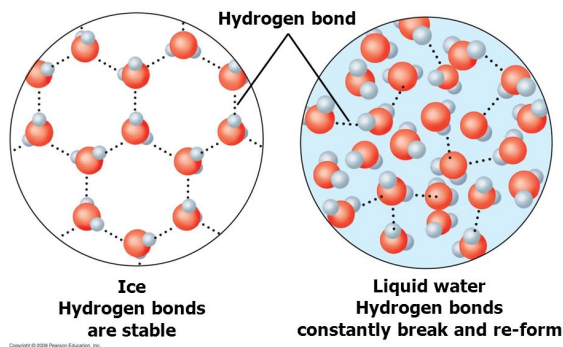


FIG. 8: Hydrogen bonds in ice and water. Image from [5].

Appendix B: Water: hydrogen bonds and ice structure

Molecules are groups of atoms that are bonded together by covalent bonds. Covalent bonds are a quantum mechanical phenomena of sharing electron pairs between atoms. In some molecules the electron pairs are more likely to be close to one atom than the other and the molecule ends up being more electronegative on one side

- the molecule is said to be polar. Water molecules and alcohols are examples of polar molecules, methane and other alkanes are examples of non-polar molecules (see Figure 9).

The slightly negatively charged oxygen of one H₂O molecule and the slightly positively charged hydrogen in another H₂O molecule tend to attract each other. This attraction, called a hydrogen bond, is typically $2-4k_B T$ (at room temperature) whereas normal attraction between non-polar molecules are typically $1k_B T$ and covalent bonds are of the order $100k_B T$.

The hydrogen bonds between water molecules cause the hexagonal ordering of ice where each molecule has a hydrogen bond to 4 neighbouring molecules. Liquid water has a similar local structure where the hydrogen bonds constantly break and reform and the water molecules on average have 3-3.5 hydrogen bonds to neighbouring molecules.

Appendix C: Equipment

1. Heat of melting

- Calorimeter
 - Stainless steel container
 - Insulation
 - Plastic lid
 - Heating element
 - Stirrer
- Power supply
- Amperemeter
- Voltmeter
- Thermometer (PASCO with USB connection to PC), to be inserted through a hole in the lid of the calorimeter.
- Digital balance
- Block of ice in water bath

2. Heat of vapourization

- Water flask with water and pebbles to nucleate vapour bubbles
- Thermometer
- Cooling element
- Heating element
- Connection with valve to vacuum pump
- Connection with valve to atmosphere

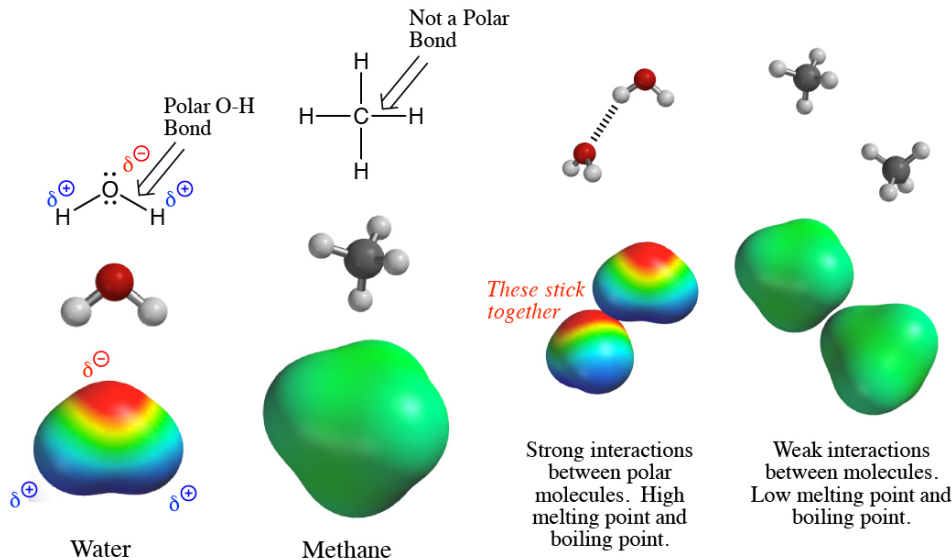


FIG. 9: Polar water and non-polar methane. Image from [1].

- Buffer volume flask
- Manometer (pressure sensor)

3. Units in the MD simulations

The MD simulations will be done with input and output in "style" *real* units that are (see <http://lammps.sandia.gov/doc/units.html>)

- mass = grams/mole
- distance = Angstroms
- time = femtoseconds
- energy = Kcal/mole
- velocity = Angstroms/femtosecond

- force = Kcal/mole-Angstrom
- torque = Kcal/mole
- temperature = Kelvin
- pressure = atmospheres
- dynamic viscosity = Poise
- charge = multiple of electron charge (1.0 is a proton)
- dipole = charge*Angstroms
- electric field = volts/Angstrom
- density = gram/cm³
- calorie = 4.184 J

- [1] B.L. Iverson. Where are the electrons. 2017. URL <http://iverson.cm.utexas.edu/courses/310N/MainPagesSp06/Whereee.html>.
- [2] David C. Johnston. Thermodynamic Properties of the van der Waals Fluid. 2014. doi: 10.1088/978-1-627-05532-1. URL <http://arxiv.org/abs/1402.1205><http://dx.doi.org/10.1088/978-1-627-05532-1>.
- [3] David A. Kofke. Direct evaluation of phase coexistence by molecular simulation via integration along the saturation line. *The Journal of Chemical Physics*, 98(5):4149–4162, 1993. ISSN 00219606. doi: 10.1063/1.465023.
- [4] Christopher O'Brien. Working with water in LAMMPS, 2020. URL <https://sites.google.com/a/ncsu.edu/cjobrien/tutorials-and-guides/working-with-water-in-lammps>.

- [5] Stackexchange. Hydrogen bonds, 2018. URL <https://chemistry.stackexchange.com/questions/96452/which-has-stronger-hydrogen-bonds-water-or-ice>.
- [6] Wikibooks. Molecular Simulation/Radial Distribution Functions, 2018. URL https://en.wikibooks.org/wiki/Molecular_Simulation/Radial_Distribution_Functions.
- [7] Wikipedia. Trouton's rule, 2019. URL https://en.wikipedia.org/wiki/Trouton's_rule.