Mathematical Modeling in Chemical Engineering

Modelling of the cooling process of an open vessel with liquid

Examination Project

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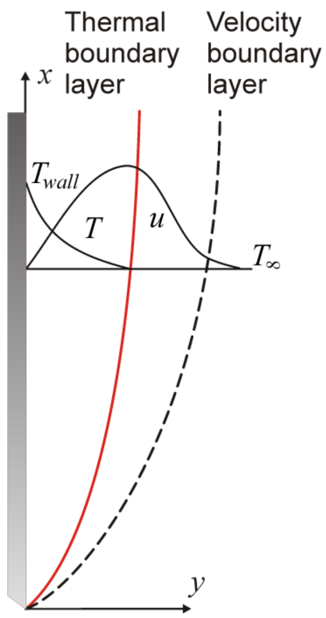
1. Project introduction and objectives

The objective of the project is to study the cooling of a vessel filled with a warm liquid. The heat transfer mechanisms shall be identified. A global model for the whole vessel and a detailed model describing the mass and heat transfer from the liquid surface shall be developed. The models are validated using measured temperatures and mass. More specific the objectives are to:

- Identify the different heat transfer mechanisms.
- Estimate how much each mechanism contribute to cooling, and how these change with time.
- Perform experiments.
- Formulate a model for the evaporative cooling mechanism.
- Estimate model parameters.
- Develop a global model that predicts how temperature and mass varies with time.
- Validate the model.
- Propose a new design of the vessel that maintain the temperature for longer time.

Heat transfer from the liquid occurs by different mechanisms i.e. free convection, evaporation and radiation. Free or natural convection driven heat transfer occurs everywhere where there is a temperature difference between a surface and a fluid. The density difference induced by the temperature gradient results in convection close to the surface.



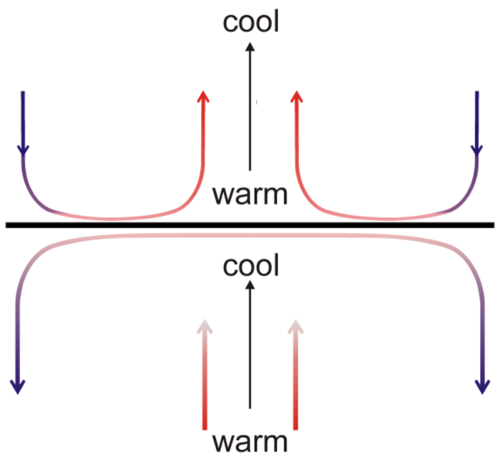


Figure 1. Free convection at a vertical surface (left) and a horizontal surface (right)

Free convection at a vertical surface is stable and very good correlations exist. Free convection at a horizontal surface is more unstable and the convection is very different for cooling and heating as well as below or on top of a surface. Cooling from a liquid surface is even more complex due to evaporation and movement of the surface due to free convection and surface tension gradients. The water vapour has lower density than air and evaporation will increase the density difference between surface and bulk. In addition the surface tension of water is temperature dependent and will induce instabilities in the surface (Marangoni effect) and increase the heat transfer mainly on the liquid side but to some extent also on the gas side.

The following sections include instructions how to formulate the model, how to collect experimental data and what should be included in the report.

2. Project prerequisites

Before you start working with the examination project you should have read the text book (*Mathematical Modeling in Chemical Engineering*), and learned how to formulate mathematical models and how to perform statistical analysis of mathematical models. It is also recommended that you have completed the tutorials. These can be downloaded at www.cambridge.org/rasmuson.

3. Project instructions

Mass and heat transfer coefficients for the vertical surfaces are obtained via Sh and Nu numbers. The correlations can be found in the literature e.g. Welty, Wicks, Wilson, Rorrer : Fundamentals of momentum, heat and mass transfer, Wiley, 2008. Correlations for physical data for water and air in the temperature interval 20–100°C are available in a Matlab file that can be downloaded from the publishers webpage.

3.1 Model formulation

Formulate mass and heat balances for the whole system. Which mechanisms are most important? Can some mechanisms be neglected? Are the mechanisms in series or in parallel?

You can use available models for free convection on vertical surfaces since they are good and reliable. However, for the horizontal surface you must develop models for Nusselt and Sherwood numbers using dimensionless numbers as described in Chapter 4 in the book. You cannot copy the models directly since the molar weight for water is less than for air and the evaporation of water introduce an additional source for the density difference between the surface and the surrounding air.

One simplification can be done if it is possible to assume that Sh=Nu. If this is possible the Nusselt number for heat transfer above the water surface can be determined independently from the total heat transfer. Motivate all assumptions that need to be made thoroughly.

3.2 Parameter estimation

Your new model for heat and mass transfer from the water surface contains unknown parameters that must be determined. Assume that existing models are sufficient for estimation of the heat flux from the remaining surfaces and estimate the Sherwood and Nusselt numbers for the water/air interface. Plot Sh/Nu versus relevant dimensionless numbers to obtain a preliminary structure of the model.

You will have measurements of both mass and temperatures and they can be used to fit the parameters. However, in this case you should only use the measured mass to obtain the parameters and use the measured temperatures to validate the model. From a preliminary guess of the unknown parameters in the model simulate how the temperature (T) and the mass (m) decreases in time and form a sum of squares.

$$SS = \sum (m_{obs} - m_{mod})^2$$

The index *obs* denote the observation and *mod* the modelled variable.

Use the Matlab routine lsqnonlin to find the parameters that minimize the sum of squares. The Matlab routine will return the sum of squares and the Jacobian that can be used to calculate the confidence intervals and the correlations between the parameters as described in Chapter 7.

3.4 Model validation

Use the model to simulate the temperature and weight decrease during the cooling. Validation of the model should be done with a new set of data that has not been used in fitting the parameters. You can also validate the developed model with data from other geometries. Also explain the differences between the observations and measured values.

3.4 Experiments

Before you start to collect data for validation, you must develop an understanding of the present system. Use smoke and dye tracer experiments to observe the flow pattern in the air and the water, as shown in Figure 2. Use the thermocouple to monitor the temperature profiles in the air and in the water. During these measurements you should identify the different cooling processes and try to quantify the impact they have on the cooling process.

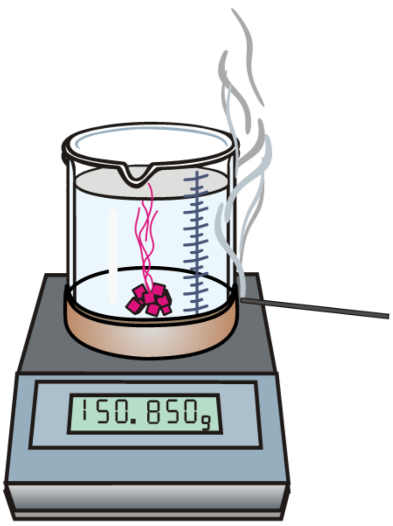


Figure 2. Experimental setup for the fluid flow visualization inside and around the beaker.

In order to increase the understanding of the cooling process and to verify the model some simple experiments are conducted. A glass beaker with hot water is placed on an insulated balance. The insulation may for example be done with Styrofoam. The temperature should be measured at different heights and at different radial locations while simultaneously measuring the mass of the liquid (see Figure 3). These measurements are done several times during the cooling process.

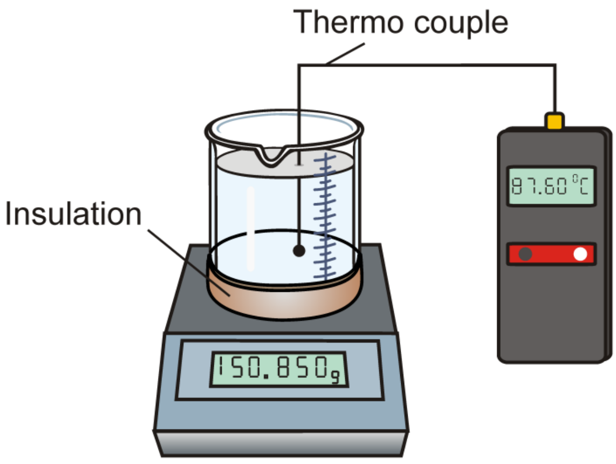


Figure 3. Experimental setup for investigating the cooling effects.

The final measurements should be done with three beakers with different volume for different groups. Temperature, mass and surrounding room temperature are monitored while the liquid temperature decreases from about 70 °C to 40 °C.

3.5 Report instructions

Write a report concluding your study. The report should include the following:

1. The global heat balance for the system.
2. The relative importance of the different heat transfer mechanisms.
3. Your model for heat and mass transfer across the water/air interface. Discuss the accuracy of the model.
4. Present your results in a graph with experimental and simulated data versus time.
5. Discuss if the assumption Nu=Sh is correct.
6. Discuss the simplifications in the model and estimate if it will lead to an under or over estimation of the predicted temperatures.
7. Discuss how fast the liquid will cool in a zero gravity environment.

Attach the MATLAB file containing your model with comments. With the use of your developed model suggest material and design of a coffee cup that should maintain the temperature of the coffee over 50 °C for as long time as possible. The volume of the cup should be 150 ml and the thickness of the wall should be maximum 5 mm.

APPENDIX A

Available correlations for heat and mass transfer

Free convection at a vertical wall:

$$Nu_L = 0.68 + \frac{0.67 Ra_L^{1/4}}{\left[1 + (0.492/\Pr)^{9/16}\right]^{4/9}} \quad Ra > 10^9$$

Free convection at a horizontal solid wall:

For a hot top surface or a cold bottom surface:

$$Nu_L = 0.54 Ra_L^{1/4} \quad 10^4 < Ra_L < 10^7$$
$$Nu_L = 0.15 Ra_L^{1/3} \quad 10^7 < Ra_L < 10^{11}$$

For a cold top surface or a hot bottom surface:

$$Nu_L = 0.27 Ra_L^{1/4} \quad 10^5 < Ra_L < 10^{10}$$

with L defined as

$$L = \frac{A_S}{P}$$

Where A_S is the surface area and *P* the perimeter