



Computational examples in transport phenomena

with Python

This document was prepared as part of two courses from Delft University of Technology: *The Basics of Transport Phenomena*, available on edX.org as DelftX: TP101x and *Advanced Transport Phenomena*, available on edX.org as DelftX: TP201x.

This material was created by or adapted from material posted on the DelftX website, delftx.tudelft.nl, and created by TU Delft faculty members Robert Mudde, Professor of Multiphase Flow at the Dept. of Chemical Engineering and Peter Hamersma, Associate Professor at the Dept. of Chemical Engineering, 2015. DelftX is not responsible for any changes made to the original materials posted on its website and any such changes are the sole responsibility of Kamila Zdybał.

The course materials by Delft University of Technology are subjected to copyright and are licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License.
<https://creativecommons.org/licenses/by-nc-sa/4.0/>

Copyright © K. Zdybał, 2018
For more projects similar to this one
visit me on GitHub: @camillejr
camillejr.github.io/science-docs/
To contact me personally drop me a line at:
kamilazdybal@gmail.com

Cover picture: *Forêt de Soignes, Belgium*
Photo taken on: 16 Jan 2017
Copyright © K. Zdybał, 2017

Computational examples in transport phenomena with Python
Typeset with \LaTeX

This work is licensed under the Creative Commons
Attribution-NonCommercial-ShareAlike 4.0 International
(CC BY-NC-SA 4.0) license.

Contents

1 General remarks on transport of physical properties	3
2 Steady-state conduction in a lengthwise-insulated rod with internal heat production	4
2.1 Final remarks	5
2.2 Computational example	5
3 Steady-state laminar flows of Newtonian fluids	7
3.1 Couette flow	7
3.2 Poiseuille flow	7
4 Lumped system analysis of a steel plate	9
5 Evaporating sphere	10
6 One-dimensional binary diffusion	11
7 The Stefan problem	12

1 General remarks on transport of physical properties

The general equation for the transport of a property ψ within a control volume is:

$$\frac{d\psi}{dt} = \Psi_{in} - \Psi_{out} + \Psi_{production} - \Psi_{consumption} \quad (1)$$

where $\frac{d\psi}{dt} = \dot{\psi}$ is the flux of the property ψ .

2 Steady-state conduction in a lengthwise-insulated rod with internal heat production

We derive a one-dimensional temperature distribution function $T(x)$ for a steady-state heat conduction in a straight rod of length L . We assume that the internal heat production Q_p in units of W/m^3 is present at every point inside the rod volume. This may for instance simulate heating up of a wire due to electrical current. The rod is perfectly insulated along its length and it loses heat only through its endpoints which in a steady-state case are kept at a fixed temperature T_0 .

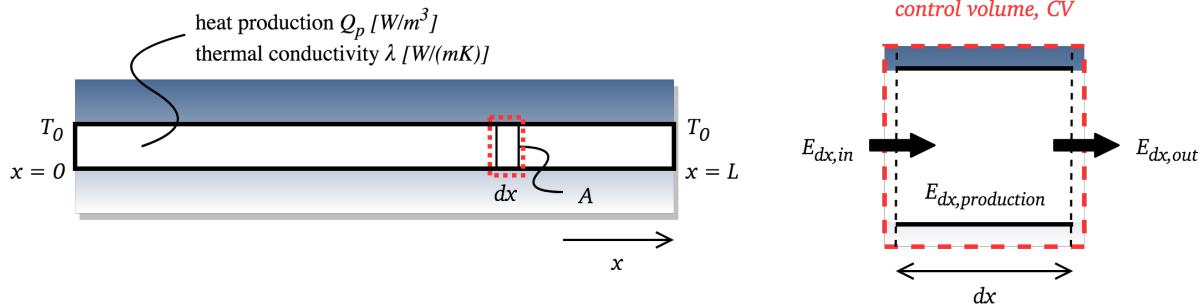


Figure 1: Conduction in a rod with internal heat production.

We will take for the control volume a slice dx from the rod. The energy balance for the rod element dx :

$$\frac{dE_{dx}}{dt} = E_{dx,in} - E_{dx,out} + E_{dx,production} \quad (2)$$

Note here that $E_{dx,in}$, $E_{dx,out}$ and $E_{dx,production}$ are energies per unit time and so have the units of W .

The heat flux ϕ which has units of W can be modeled using the Fourier's law for one-dimensional heat conduction:

$$\phi = \lambda A \left(-\frac{dT}{dx} \right) \quad (3)$$

where λ is the thermal conductivity and is a property of the material, A is the rod's cross-sectional area and $\frac{dT}{dx}$ is a temperature gradient which plays a role of the driving force for thermal energy transport.

Hence:

$$E_{dx,in} = \lambda A \left(-\frac{dT}{dx} \right)_x \quad (4)$$

$$E_{dx,out} = \lambda A \left(-\frac{dT}{dx} \right)_{x+dx} \quad (5)$$

The energy per unit time coming from the heat production can be written as Q_p multiplied by the volume of the slice dx :

$$E_{dx,production} = Q_p A dx \quad (6)$$

In the steady-state $\frac{dE}{dt} = 0$ and the energy balance becomes:

$$\lambda A \left(-\frac{dT}{dx} \right)_x - \lambda A \left(-\frac{dT}{dx} \right)_{x+dx} + Q_p A dx = 0 \quad (7)$$

Simplifying the above energy balance we get:

$$\frac{\left(\frac{dT}{dx}\right)_{x+dx} - \left(\frac{dT}{dx}\right)_x}{dx} = -\frac{Q_p}{\lambda}$$

It is interesting to note here that we have lost the dependence on the cross-sectional surface area of the rod.

If we now substitute some function $f(x) = \frac{dT}{dx}$ we notice that we have:

$$\frac{f(x+dx) - f(x)}{dx} = -\frac{Q_p}{\lambda}$$

in other words:

$$\frac{df(x)}{dx} = -\frac{Q_p}{\lambda} \quad (8)$$

With the above substitution, the differential equation that we are about to solve becomes:

$$\frac{d^2T}{dx^2} = -\frac{Q_p}{\lambda} \quad (9)$$

Applying the boundary conditions from both ends of the rod, the solution to the above differential equation is:

$$T(x) = -\frac{Q_p}{2\lambda}(x^2 - Lx) + T_0 \quad (10)$$

2.1 Final remarks

Note that even though the heat flow was assumed to be one-dimensional in this exercise, it does not mean that the geometry of the problem needs to be one-dimensional. In fact, we assumed the rod to be a three-dimensional object having length and a cross-sectional area. Rather, the one-dimensionality of the problem means that it is practical to assume only one of the three directions as an important direction for heat transport. Since the rod was perfectly insulated along its length, the temperature gradient along directions perpendicular to the x -axis is zero.

2.2 Computational example

As a computational example we will draw the graph of the temperature distribution in a copper rod 200m long. We assume that the thermal conductivity for this rod is $400 \frac{W}{m \cdot K}$. The internal heat production in the entire rod is 20W.

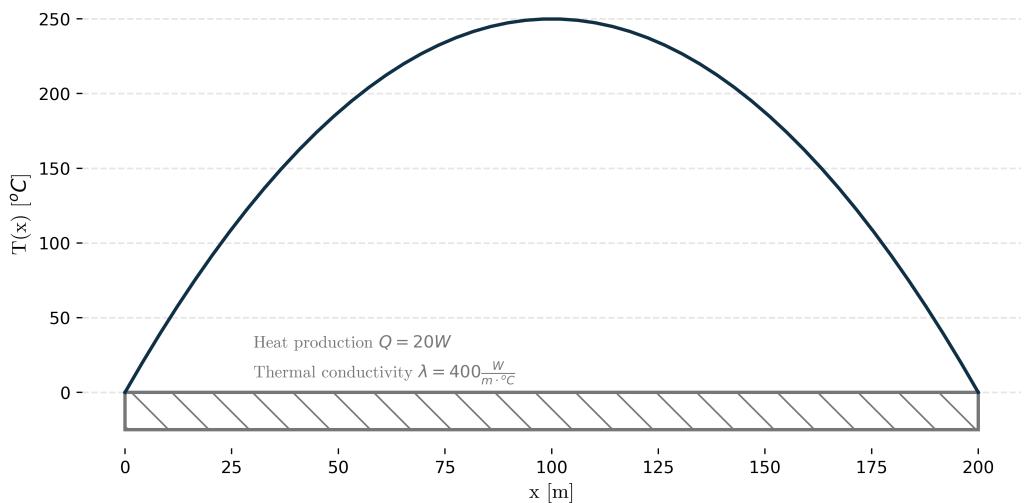


Figure 2: Temperature distribution in a rod with internal heat production of 20W.

3 Steady-state laminar flows of Newtonian fluids

The derivation of the velocity distribution in a steady-state laminar flow of a Newtonian fluid starts with writing the equation for momentum transport between the fluid *laminates*.

3.1 Couette flow

3.2 Poiseuille flow

Consider a steady-state flow of fluid between two parallel plates. We would like to find the velocity and shear stress distribution along the y -axis. The pressure drop is assumed to be constant throughout the channel. This means that the pressure is a function of position $p = p(x)$ but the change in pressure per every equal distance in the channel is constant: $dp/dx = \text{const}$. The width of the channel B is much larger compared to its other dimensions.

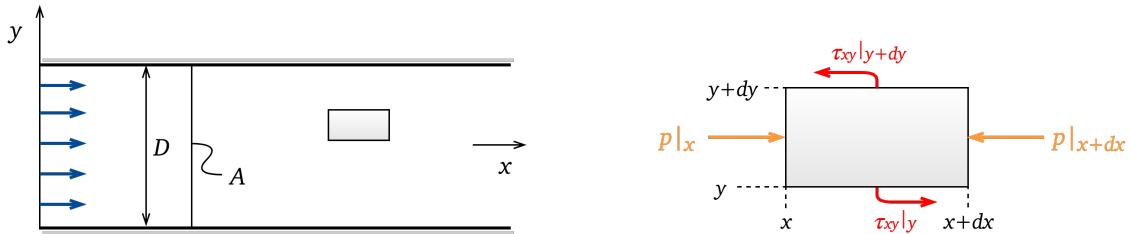


Figure 3: Flow between two parallel plates with an infinitesimal fluid element.

We also have three boundary conditions. Due to a no-slip condition we assume that the velocity at the very surface of the plates is zero: $u(-D/2) = 0$ and $u(D/2) = 0$. Due to symmetry of the flow we assume that there cannot be any net momentum transfer between the upper half and the lower half of the channel. Hence, the shear stress exactly in the middle of the channel is zero: $\tau_{xy}(0) = 0$.

Steady state momentum (force) balance, taking into account pressure and shear forces on a single infinitesimal fluid element:

$$0 = p|_x B dy - p|x+dx B dy + \tau_{xy}|_y B dx - \tau_{yx}|_{y+dy} B dx \quad (11)$$

Dividing both sides by the width B and by $dx dy$ we obtain:

$$0 = \frac{p|_x - p|x+dx}{dx} + \frac{\tau_{xy}|_y - \tau_{yx}|_{y+dy}}{dy} \quad (12)$$

Now we notice that $\frac{p|_x - p|x+dx}{dx}$ is in fact equal to $-\frac{dp}{dx}$ (in a limit as $dx \rightarrow 0$), since it is an incremental change in pressure function value per incremental distance dx . Similar thing can be said about $\frac{\tau_{xy}|_y - \tau_{yx}|_{y+dy}}{dy}$ which is equal to $-\frac{d\tau_{xy}}{dy}$. We can thus further simplify:

$$\frac{d\tau_{xy}}{dy} = -\frac{dp}{dx} = \text{const} \quad (13)$$

Integrating the above equation and applying the initial condition for the shear stress $\tau_{xy}(0) = 0$:

$$\tau_{xy}(y) = -\frac{dp}{dx} y \quad (14)$$

Adding a constitutive relation for Newtonian fluids we can further relate pressure and velocity. From the Newton's law we know also that:

$$\tau_{xy}(y) = -\mu \frac{du}{dy} \quad (15)$$

You may look at this in such a way: the equation 14 is a special case in which the shear stresses have been related to the driving force in the Poiseuille flow - the pressure gradient. The equation 15 is a general description of any shear stress τ_{xy} , where it is linked to velocity gradients, no matter what the cause for this velocity gradient is! It just so happens that in the case of a Poiseuille flow between two parallel plates this cause is the pressure drop:

$$-\mu \frac{du}{dy} = -\frac{dp}{dx} y \quad (16)$$

Integrating one more time the above relation and applying the no-slip boundary conditions we get:

$$u(y) = \frac{1}{2\mu} \frac{dp}{dx} (y^2 - (D/2)^2) \quad (17)$$

4 Lumped system analysis of a steel plate

5 Evaporating sphere

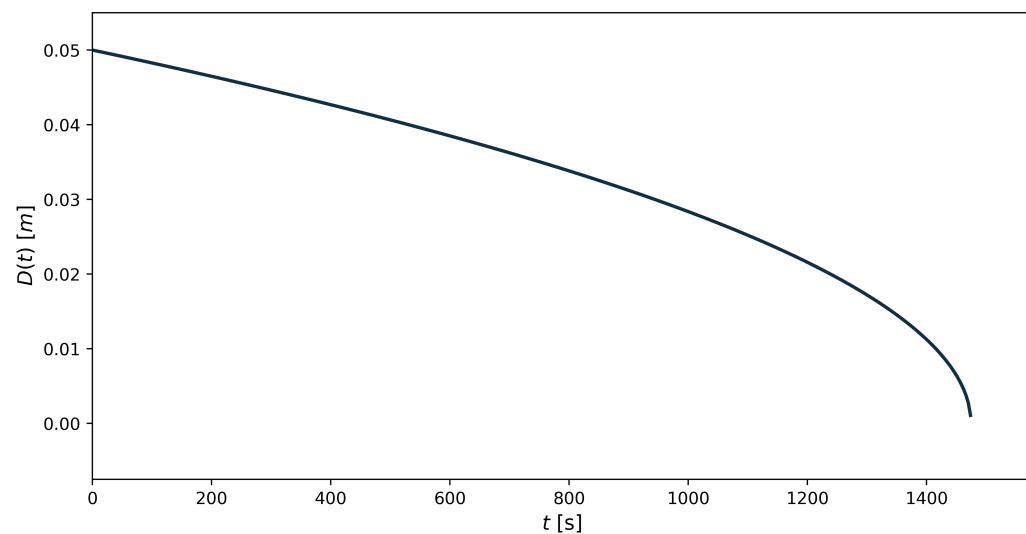


Figure 4: Evaporating sphere diameter history.

6 One-dimensional binary diffusion

7 The Stefan problem

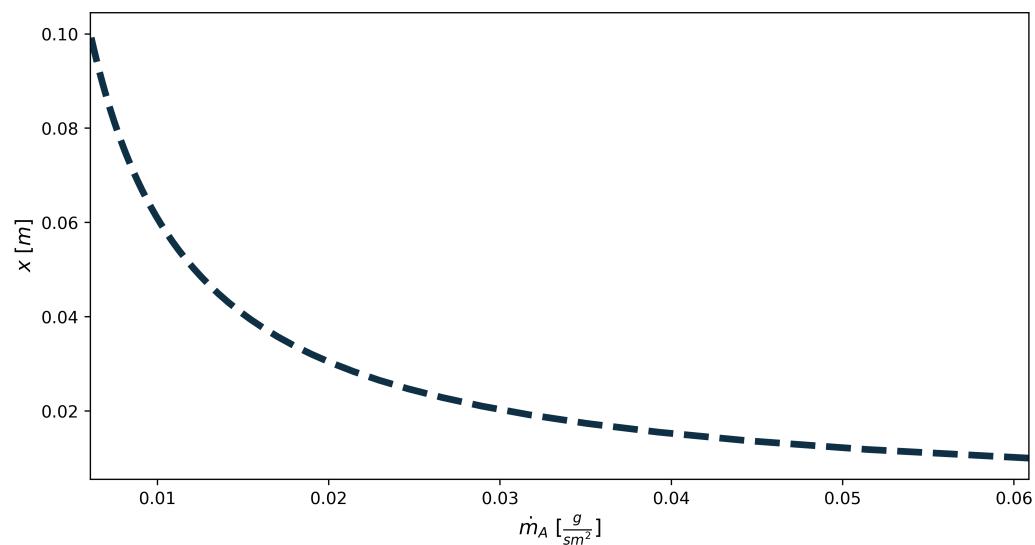


Figure 5: Stefan problem for water evaporating from the 0.1m tube.