Project work for TMA4212

Rubber Vulcanization

Physical problem

Vulcanization is a chemical process used to cross-link rubber polymers (typically with sulfur) in order to improve mechanical strength and elasticity. During production, a rubber component is placed in a heated mold. Heat diffuses into the material and triggers an exothermic chemical reaction. The heat released by the reaction further increases the temperature, creating a nonlinear coupling between heat transfer and reaction kinetics.

The purpose of this project is to model and simulate this process using finite difference methods.

Mathematical Model

We model:

- $T(x,t)$: temperature [K]
- $\alpha(x,t)$: degree of cure (0 = uncured, 1 = fully cured)

The temperature is described by the heat equation with a reaction source term:

$$\rho c_p \frac{\partial T}{\partial t} = k\Delta T + \rho H_r \frac{\partial \alpha}{\partial t} \qquad \text{on } \Omega. \tag{1}$$

The heat is transferred to the rubber object by convection at the boundary, described by

$$-k\frac{\partial T}{\partial n} = h(T - T_m) \quad \text{on } \partial\Omega. \tag{2}$$

where T_m is the mold temperature. The cure kinetics is given by the Arrhenius Law, that is

$$\frac{\partial \alpha}{\partial t} = \begin{cases} 0 & T \le T_s \\ A\exp\left(-\frac{E}{RT}\right)\alpha^m(1-\alpha)^n & T > T_s \end{cases} \tag{3}$$

thus curing starts first when the temperature has reached some treshold temperature T_s.

A set of model parameters are given in Table 1. pe

density	ρ	$= 1100$ kg/m^3	pre-exponential factor	A	$= 5 \times 10^5$ s^{-1}
heat capacity	c_p	$= 1900$ J/(kg K)	activation energy	E	$= 8.0 \times 10^4$ J/mol
thermal conductivity	k	$= 0.2$ W/(m K)	gas constant	R	$= 8.314$ J/mol K
total reaction heat	H_r	$= 2.5 \times 10^5$ J/kg	reaction exponents	m	$= 1.2,\ n = 1.8$
heat transfer coefficients	h	$= 200$ W/(m^{2}K)	treshold temperature	T_s	$= 393$ K

Table 1: Representative model parameters

Task 1:

Rewrite the model in dimensionless form. The following scalings are suggested:

$$\begin{aligned}
&\text{Temperature scaling:} && u = \frac{T - T_0}{T_m - T_0}, \\
&\text{Space scaling:} && x^* = x/L, \\
&\text{Time scaling:} && t^* = t/t_{\text{diff}}, \quad t_{\text{diff}} = \frac{\rho c_p L^2}{k}.
\end{aligned}$$

Here L is a representative size for the rubber object, and T_0 is the initial temperature.

Rewrite the system using these scalings, and identify the most important dimensionless parameters. These parameters determine the qualitative behavior of the system.

Notice that $u(x, 0) = -1$.

Task 2:

Solve the heat equation numerically on a two-dimensional square domain

$$\Omega = [0, L] \times [0, L], \qquad L = 2 \text{ cm}.$$

As initial values for the temperature, use $T_0 = 300$ K. The mold temperature is $T_m = 443$ K.

Use a 5-point discretization for the discretization in space. Choose some appropriate discretization in time.

Show consistency and (von Neumann) stability of your chosen scheme (no details in the slides, just the results). Justify theoretical results by numerical experiments.

Task 3:

Include the reaction term.

There are several options for doing this. One possibility is to use a splitting scheme: Do one step for the heat equation, and then one step for the reaction term, using the updated temperature. Whatever you choose, your choice should be justified.

When you have a running code: consider the following:

- Development of temperature and curing over time (make some snapshots).
- Degree of cure in the center.
- Time to reach 90% cure in the center.
- Maximum temperature inside the square. Does it exceed the mold temperature (overheating)? If yes, where?

Hint: In order to get the curing started, you need to set some small value for $\alpha(0)$.

Task 4:

In this task, you are free to investigate the problem further, in a direction of your own choice. The final grade will depend on extent, complexity and quality of your investigations.

Some ideas:

- Parameter studies: Study the effect of changing parameters. The most interesting here might be the heat transfer coefficient h and the activation energy E (or better, the relevant dimensionless parameters). Can you find some tresholds for overheating?
- Extend the problem to 3D.
- Choose a more complicated geometry of your object.

- For the more theoretical inclined: Consider a linear simplified curing law:

$$\frac{\partial \alpha}{\partial t} = \begin{cases} 0 & T \leq T_s \\ \lambda(T - T_s) - \gamma\alpha & T > T_s \end{cases} \tag{4}$$

  and do some theory on the linear system.

Submission

- Well-documented source code. It should include a `readme`-file, describing exactly how to run the code. A Jupyter notebook is an alternative. The code should run on a mac computer, without any modifications!
- Slides for a 10 minutes presentation (pdf or powerpoint).

  The presentation should clearly present the mathematical model, the numerical method, and a discussion of the results. In the slides all parameteres used in the simulations should be spesified. Give most emphasis to Task 3 and 4.
- A separate sheet stating clearly how generative AI has been used (if at all), and which tools you have used.