Shape Optimization in Phosphate Production

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Phosphate as an industrial product is an essential ingredient in, e.g., agriculture and food industry. The production process is very energy consuming and takes place in high temperature melting furnaces. The costs of the productions are largely governed by the energy costs of the furnace and there is a high potential to save energy by increasing its energy efficiency. Naturally, the shape of the furnace has a high influence on its efficiency. In order to describe the temperature distribution within a furnace mathematically, a widely used model in the industry is the Rosseland approximation. We use this model and discuss the problem in the context of shape optimization.

1 Introduction

In the context of energy transition in Germany it is essential to consider every source of potential energy savings. In 2016 the amount of energy needed in form of heat was about 4933 Petajoule. The dominating areas are processes in the industry, with 1713 Petajoule, and private households, who need 1664 Petajoule to heat their rooms.¹ It is apparent that there is a large potential to be exploited in the industrial sector. There, high temperature processes require a lot of energy to guarantee a certain level of product quality. In the following we look at phosphate production as an example of such a process and investigate how the shape of the furnace effects the heat distribution within the furnace. We apply tools from shape optimization to find a shape which increases the efficiency of the furnace which results in energy savings.

2 Approximation of the Multi Physics Problem

Phosphate production, in a nutshell, works as follows: Neutralized phosphoric acid flows into the furnace and gets heated up by the flame. If it is hot enough phosphate is created as the result of an endothermic reaction. The final product flows out on the other side of the furnace. To model the whole process one has to consider heat transfer and flows in the atmosphere and in the liquid and find coupling conditions between both domains. Additionally the chemical reaction has to be modelled. Simulating such a process is computationally very challenging, especially in the context of optimization. To start with a simple framework we only model the atmosphere and simulate a two dimensional front view of the furnace. Furthermore we omit convection and only consider heat transfer given by conduction and radiation which on the kinetic level still results in a five dimensional equation, see [5]. An approximate model to describe heat transfer often used in an industrial context is Rosseland’s Approximation, see [1]. Equipped with boundary conditions of Robin type, which induce a cooling at the boundary, the scaled equation reads

\[-\nabla \cdot \left( k + \frac{16\pi a}{3\kappa} T^3 \nabla T \right) = f \text{ on } \Omega, \]

\[k \nabla_n T = h(T_b - T) \text{ on } \partial \Omega,\]

where we used the following scaled constants:

\[T_b \quad \text{Temperature outside} \]
\[k \quad \text{Heat conductivity coefficient} \]
\[h \quad \text{Convective heat transfer coefficient} \]
\[a \quad \text{Stefan Boltzmann constant} \]
\[\kappa \quad \text{Absorption coefficient} \]

Here we use a stationary model, which is motivated by the fact that the furnace runs continually the same way at any time.

3 Shape Optimization

The mathematical optimization problem reads

\[\min_{\Omega} J(\Omega) = \min_{\Omega} \int_{\Omega} \left| T_{\Omega} - T_d \right|^2 dx,\]

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¹ https://www.umweltbundesamt.de/bild/waermebedarf-der-sektoren-nach-anwendungszwecken

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where $T_\Omega$ solves Equation (1) on the domain $\Omega$. Here, $\Gamma_B$ represents the bottom of the furnace where we require a certain temperature $T_d$ in order for the chemical reaction to take place. To calculate the shape derivative we use a Lagrangian ansatz according to [4] and to compute the gradient we use the equations of linear elasticity. To get smoother transformations within the domain and to avoid degenerate elements we follow the approach presented in [2] and use a stiffness function which solves a Laplace equation.

4 Numerical Results

To perform the optimization we use an implementation of a standard gradient method, where we iterate until relative changes are small. We determine the step size used in the transformation step according to an Armijo rule with the additional constraint that the mesh does not become degenerate. The implementation was done in Python 3.6.5 using FEniCS 2017.2.0.

As an initial domain $\Omega_0 = [0, 1] \times [0, 0.5]$ is used for all test cases. We further aim to attain a desired temperature profile of constant $800 K$ at $\Gamma_B$. The following results were produced using the physical parameters $a = 5.67 \cdot 10^{-8}$, $h = 1.4$, $\kappa = 3$, $k = 20$, $T_b = 300$. The flame can be modeled as the solution to an inverse problem, see [3].

We look at two test cases. In test case a) we allow for arbitrary perturbations, whereas in case b) we only consider shapes which result as perturbations into the $y-$ direction. In each case the bottom of the furnace $\Gamma_y$ is stationary. Case b) may be interpreted as the “industrial case”. The real world furnace is surrounded with a cooling mechanism and therefore variations in height and changes of the vault are easier to realize. In both cases we look at two settings determined by the value of the constant $c$, i.e., how hot the flame is. We choose $c_s = 6600$ to represent the setting where the initial temperature distribution is below $T_d$ and $c_l = 33000$ to get an initial distribution which is mainly above $T_d$. Each setting results in a different behaviour of the optimization.

From Figures 1-3 the limits of this model become evident. Starting with $c = c_s$ the optimal furnace grows in size, independent of the choice of admissible shapes.

Due to the lack of boundary radiation effects contained in the model the boundary is only seen as a heat sink which should be far away from $\Gamma_B$. The case where $c = c_l$ confirms this. We see that the cooling effect of the boundary is used to cool the interior of the domain. It is additionally used to cut out parts of the flame to reduce the energy entering the system.

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