The Impact of Mathematical Modeling on the Production of Special Purpose Cement

Domenico Lahaye and his helping friends

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Introduction

What impact can mathematical modeling have in the production industry? Our partnership with Almatis B.V., a special purpose cement manufacturer, resulted in the complete elimination of unscheduled plant shut-downs. Almatis now reports a much more stable manufacturing process and hence a very significant productivity increase. The key to our success resides in the deployment of advanced computational fluid dynamics techniques. It is currently driving a long-term collaboration expanding into different branches of Almatis. Students employed on the project can train in the mathematical modeling of turbulent combustion, granular material flow and material phase transformations. They are offered the opportunity to experiment with modern simulation software on parallel hardware and to interact with experts in various engineering disciplines.

Production of Special Purpose Cement

Commonly used cement is easy to manufacture. A long cylindrical rotating furnace or *kiln* is typically employed in the process. I have schematically represented the production process in Figure 1. Cement kilns are slightly tilted to facilitate the lateral downward motion of the material. As the kiln rotates in its axis, the powder material traverses the furnace from the inlet to the outlet. It is being mixed and heated up to a sufficiently high temperature. These processes cause the reactions that transform the raw materials into the final product.

However, the special purpose cement produced by Almatis (www.almatis.com) requires processing the mixture of a calcium-bearing limestone and an aluminum-bearing material at high temperature. This requires the control of the critical process parameters such as the temperature inside the oven and its rotational speed. Experience at the Almatis plant in Rotterdam has shown that neither trial and error nor empirical modeling provide sufficient insight into these critical conditions. Measuring the temperature inside the kiln has proven to be difficult due to the harsh operating conditions. Without accurate temperature readings, the amount of heat absorbed by the material remains hard to track. The stringent product quality specifications imposed by Almatis are therefore hard to attain. The efficiency of the kiln is doomed to remain suboptimal. As a world-leader in calcium-alumina special purpose cement, Almatis is eager to invest in research partnership and to use cutting edge technologies. This will allow to better serve various industries that rely on Almatis cement in applications exposed to high temperature.

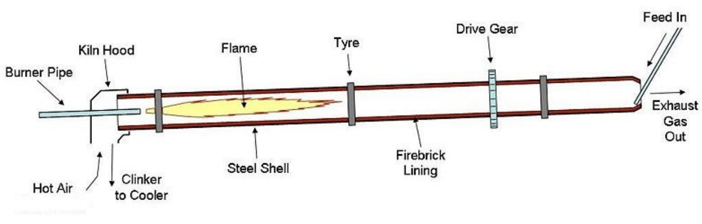

Figure 1: General layout of a rotary kiln used at Almatis and modeled by the scientific computing group.

The scientific computing group developed a detailed mathematical model that accurately predicts the temperature, the radiative heat distribution, and the absorption of heat by the material bed inside the oven. The use of advanced computational fluid dynamics techniques proved to be vital. In the next sections, we will describe the mathematical models and the results obtained in some more detail.

Mathematical Modeling

Michele Pisaroni and Miguel Romero built the mathematical model of the rotary kiln in use by Almatis at their plant in Rotterdam during their master degree. They executed the project in two stages. In the first stage, Michele relied on the fact that only a small fraction of the space inside the kiln is taken up by cement material. This allowed him to assume the kiln to be empty and to develop a three-dimensional non-premixed turbulent combustion model that predicts the temperature and radiative heat profile distribution inside the kiln. In the second stage Miguel built upon Michele's results and constructed a system of coupled ordinary differential equations for the absorption of heat by the material as it traverses through oven and for the ensuing phase transformation and chemical reactions. The combination of the two models provided Almatis with a better grip on its production process.

Modeling Turbulent Combustion

Combustion [3] is the physical process in which fuel and air mix and chemically react. This reaction produces heat and combustion products such as water and carbon-monoxide. Describing combustion requires capturing both the flow phenomena and the chemistry involved. In our case, the combustion is fed by an inflow of natural gas and air through distinct channels in the burner pipe shown to the far left of Figure 1. Fuel and air reach the combustion area prior to being mixed. The amount of inflow of fuel and air and heat generated cause the flow to quickly exceed the laminar regime and to become turbulent. The combustion is said to be a non-premixed turbulent combustion.

Turbulent combustion is difficult to model due to its chaotic flow pattern. A sufficiently accurate description is, however, indispensable in quantifying the mixing of fuel and air as well as the intensity of the chemical reactions. The occurrence of turbulence, in particular, enhances the mixing. Adding to the difficulty is the fact that the heat released by the chemical reactions, in turn, strongly affects the turbulent flow.

Numerical simulations environments capture turbulent combustion by imposing the conservation of mass, momentum and energy of the individual species in the reacting flow. This leads to the set of Navier-Stokes equations to which a model for the combustion and the turbulence is added. These set of partial differential equations is discretized by a finite volume method on an unstructured polyhedral mesh and solved by multigrid preconditioned Krylov methods.

A sample result of the computations by Michele Pisaroni is given in Figure 2. This figure shows the temperature along the axis of the kiln for two operating conditions differ in the amount of air used. The increase of the amount of air reduces the expected peak temperature. The location of the peak temperature and the amount by which it is reduced could, however, only be revealed through numerical simulation.

Modeling Material Processing

Miguel Romero constructed a mathematical model for the processing of the granular materials inside the kiln. He first quantified how the rotary motion of the kiln around its inclined axis causes these materials to mix and to flow in axial direction. To this end, he studied both discrete element methods [4] as well as extensions of the Navier-Stokes equations that takes two phases (solid and air) into account. Next, he identified the different paths and mechanism for the heating up of the materials. Both the shell surrounding the kiln and the air-gas mixture flowing inside it transmit heat to the materials via diffusion, convection and radiation. In the final stage Miguel linked the temperature of the mixture of materials to the chemical reactions and to the phase transformations. The model he constructed predicts the position, temperature and amount of liquid fraction of an infinitesimal amount of mixture of the granular material as it traverses the kiln. This amount of liquid fraction is a reliable indicator of the quality of the final cement product. The model requires as input the temperature and the radiative heat distribution computed by Michele at an earlier stage.

Miguel's model explains how the difference in the temperature profiles shown in Figure 2 affects the liquid fraction and therefore the quality of the end product. Data recorded at the Almatis plant in Rotterdam has repeatedly shown that the model makes accurate predictions. Such data is shown in Figure 3. This figures shows how the produced amount of material A, B and C meeting the stringent quality requirement has significantly increased after changing the temperature profile.

During the course of their work Michele and Miguel had ample opportunities to interact with and to learn from leading experts in combustion and granular flow. Michele travelled to London for a training in the simulation software he has been using, while Miguel extensively discussed his work with a senior scientist at the CSIRO in Camberra, Australia. Their work resulted in numerous conference contributions and two journal articles [2, 5]. A video highlighting the collaboration between the scientific computing group and Almatis is available at the website [1]. Michele is currently persuing a PhD at the EPFL in Lausanne, and Miguel holds a research position at BASF in Ludwigshafen.

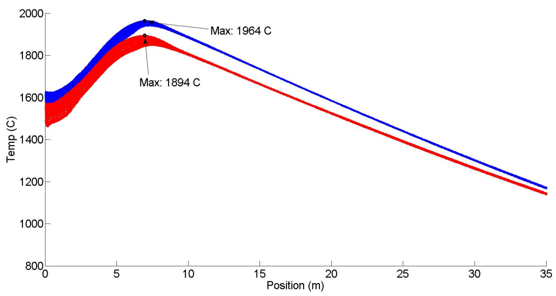

Figure 2: Computed temperature profiles along the axis of the kiln for two operating conditions.

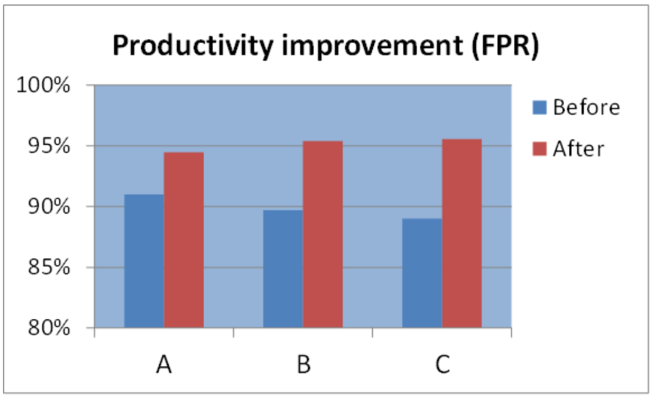

Figure 3: Measured productivity increase for the product A, B and C

Future Challenges and Opportunities

The impact of the work of Michele and Miguel is driving Almatis to further invest in the collaboration with the scientific computing group. Many questions on the operation of the rotary kiln remain unanswered. Almatis is eager to invest in more research on combustion to render the process more fuel efficient and more environmental friendly. Further research into the mixing of the granular material processing is indispensable in meeting the ever growing demands of the customer. Almatis is looking for a PhD student willing to take up these challenges.

Research has furthermore, expanded into the modeling of so-called vertical shaft kilns operated by Almatis. In these kilns the reinforcement for the high quality cement is produced. Two students, Lu Cheng and Bonnie Fan, have worked on the combustion modeling and the material processing in these kilns, respectively. Unlike the cement kiln, this kiln is completely filled by the material and the two processes cannot be decoupled. Almatis has student internships available to model the shaft kiln in a fully coupled manner.

The partnership between Almatis and the scientific computing group is awaiting a bright future and invites motivated students to contribute to the success story.

References

[1] D. J. P. Lahaye. Almatis TU Delft promotion video: www.youtube.com/watch?v=AxifpqOLPMQ.

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