Perfecting the chocolate-making process

The crystallisation of chocolate during the manufacturing process is vital to the characteristics of the final product. **Professor Thomas Hocker** describes how computer modelling methods have been used to optimise crystal formation in chocolate in order to improve the manufacturing process and create the perfect end result

Can you explain how your research background has equipped you to study the science of chocolate making? What do you enjoy most about chocolate research?

I am a chemical engineer specialising in the modelling of thermodynamic processes and phenomena. I previously worked on fuel cells, which required a joint focus on models and experimental data, and close interactions with researchers from different disciplines. This experience encouraged me to start working on the theory of chocolate making. In the beginning it was quite tough, and it took us more than a year to even begin developing our first computer models. Fortunately, we discovered that traditional chocolate researchers often have a similar attitude to us: a passion for improving something that's already very good and an acute attention to detail. This attitude is highly motivating to me.

Why is it so difficult to model the behaviour of chocolate during its production process?

How chocolate crystallises when going from liquid form to solid state is essential for the features of the final product. This process influences how chocolate melts in the mouth and hence how the flavours are released, as well as its gloss, snap and storage life. Cocoa butter is the main ingredient in chocolate and can exist in at least five different crystal forms – some of which are desired and some of which are not. The crystal formation depends on equilibrium thermodynamic behaviour and kinetic phenomena, both of which are difficult to model. In addition, the process conditions under which chocolate is made in industry are often poorly understood.

How does your research overcome the challenges associated with the conventional chocolate optimisation method?

Chocolate is usually characterised using laboratory equipment under ideal conditions, and often it is not clear how closely these conditions mimic the real production process. Therefore, our approach to making better chocolate has both an experimental and a theoretical element. On the one hand, we use sophisticated inline measurements to monitor the crystallisation behaviour of chocolate under real production conditions and, on the other hand, we use these data to validate our computer models, which then can be used to explore different optimisation scenarios.

What is unique about the combination of theoretical and experimental methods you use in your research on chocolate crystallisation?

The commerical products used by chocolate makers for inline measurements did not meet our requirements, so we had to develop our own hardware. For example, we developed our own data logger the size of an iPhone to record temperatures and heat fluxes while the chocolate moulds travelled through the cooling tunnels. We also found that the placement of the sensors sometimes caused unacceptable measurement errors, so we used computer models to find the correct positions. With respect to modelling, we characterised the crystallisation behaviour of chocolate products based on differential scanning calorimetry data. We then used the crystallisation model to predict the time- and position-dependent solidification of chocolate under conditions similar to those seen in the commercial process.

In what way does cross-disciplinary collaboration play an important role in your research?

Before we could start developing new models, we had to understand the experiences and ideas of food engineers. We cross-checked their findings and opinions with what had been published; all models need experimental data to specify input parameters and it is important to fully understand how these data were obtained, including possible uncertainties and sources of error. So far, we can demonstrate that our models provide meaningful results, but we have yet to make sure they are implemented in the best way. This again will require close interaction with R&D departments at chocolate manufacturing companies. So, cross-disciplinary collaboration is essential during all stages of the development process.

To what extent do you anticipate your projects will have a beneficial impact on companies in the chocolate industry?

I believe our research will help the companies speed up their optimisation tasks. It could be as simple as making maximum use of the experimental tools to perform inline measurements and adjust the operation parameters of existing process equipment accordingly. Or, in the long run, it could involve designing new and improved equipment by making maximum use of our models.

How computer models are helping to manufacture tastier chocolate

The difficulty of developing models of the chocolate manufacturing process has recently been overcome by a collaboration between chocolate-making company **Felchlin**, the **Swiss Federal Institute of Technology Zürich** and the Institute of Computational Physics at **Zürich University of Applied Science**, Switzerland, by successfully integrating experimental data with theoretical models

WE ALL HAVE our favourite brands of chocolate, but good quality chocolate is not an entirely subjective matter. It can be measured by the melting point in the mouth (the lower the better), how the chocolate feels once it has melted (smooth and silky rather than gritty) and the intensity of flavour (intense and not too sweet).

As Professor Thomas Hocker from the Institute of Computational Physics at Zürich University of Applied Science explains, the quality of chocolate depends "not only on the ingredients used, but also on the way in which the ingredients are processed". Crucially, chocolate can crystallise in six different crystal forms – and the crystal composition of chocolate has a big impact on its taste, how it feels in the mouth, how it snaps and the length of its storage life. During chocolate production, properly regulated heating and cooling cycles (via processes known as tempering or, alternatively, the seeding of stable crystals), together with the final cooling process, are critical for obtaining the right types of crystals – that is, stable crystals – to create high-quality chocolate.

ASSESSING THE QUALITY OF CHOCOLATE

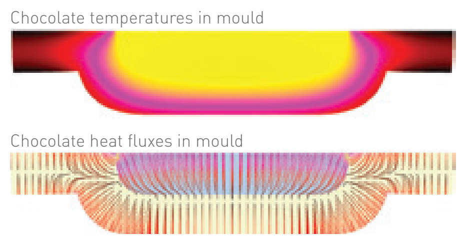
The quality of chocolate is usually monitored by measuring the temporal evolution of the chocolate temperature during the solidification process to plot a cooling curve. This can be used as a 'fingerprint' for both the used raw materials and the manufacturing process; the shape of the cooling curve gives hints about the taste, mouthfeel and storage life of the final product.

However, the problem with obtaining cooling curves in the laboratory lies in the fact that the cooling conditions used in lab equipment differ from those in commercial manufacturing cooling tunnels. The results obtained under laboratory conditions cannot easily be transferred to the real world, meaning that laboratory tests fail to show how to best optimise the commercial production process of chocolate.

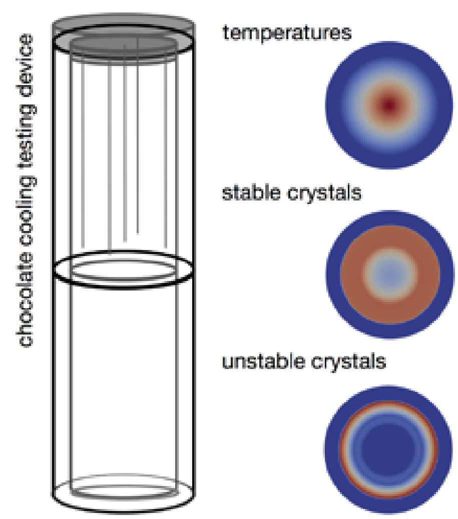
THE IMPORTANCE OF COLLABORATION

A collaboration between the chocolate maker Felchlin (represented by Manfred Suter), Eidgenössische Technische Hochschule Zürich (represented by Professor Erich Windhab) and the Institute of Computational Physics at Zürich University of Applied Science (ICP–ZHAW – represented by Hocker) has developed computational models to predict the crystallisation of chocolate and improve the commercial chocolate manufacturing process.

Suter, a food engineer employed by Felchin and originally a chef, was looking for a Master's programme in 'multiphysics' to inspire him with a new methodology and fresh ideas. Through



Computer simulations predicting how the heat is released from the chocolate upon cooling.



Computer simulations by Dr Yasser Safa predicting the crystallisation behaviour of cocoa butter.

APPLYING COMPUTER MODELLING METHODS TO THE CHOCOLATE MAKING PROCESS

OBJECTIVE

To develop computational models to predict the crystallisation of chocolate and improve the commercial chocolate manufacturing process.

KEY COLLABORATORS

Dr Peter Braun, Swiss Food Research, Switzerland

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THOMAS HOCKER is a chemical engineer who received his PhD at Johns Hopkins University, USA, in the field of statistical thermodynamics. After a postdoc position at ETH Zurich, Switzerland, he joined Zurich University of Applied Science in Winterthur, Switzerland, in 2002. He currently holds a faculty position there in computer modelling and has led the Institute of Computational Physics for the past five years. His research centres on applied thermodynamics, focusing on fuel cells and food processing.

Zurich University of Applied Sciences
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an internet search he found ICP–ZHAW and Hocker. Unlike many of his colleagues, Hocker quickly developed a curiosity about the world of chocolate making. Traditionally a purely empirical art, it seemed at first sight a completely different ball game to the theoretical world of computational physics. However, it soon became obvious that Hocker and Suter shared a similar curiosity and passion for research, combined with an acute attention to detail – and their initial discussions turned into an exciting and ambitious research project.

The beginning of the collaboration was far from straightforward, though. Modelling the crystallisation of chocolate turned out to be a vast and almost impossible task, mainly because the raw ingredients of chocolate (cocoa butter, cocoa solids, sugar, vanilla and milk) exhibit variability in their complex physical-chemical properties. By the end of the first year of working together, they were close to giving up on the project.

Fortunately, it was at this point that Hocker and Suter made contact with Professor Windhab, an expert in the rheology of food materials and a leading researcher in the field of chocolate making. He encouraged Hocker and Suter to focus on the crystallisation of chocolate by applying combinations of different theoretical and experimental methods. Vitally, Windhab also had well-established research collaborations with numerous Swiss chocolate companies. Twice a year, results from different research projects, and ideas for new projects, are disseminated through meetings held by Arbeitskreis Schoko, the Swiss working group on chocolate. This forum has existed for 20 years and it stimulates the exchange of information and ideas between developers from different chocolate companies.

MAKING BETTER CHOCOLATE

In chocolate manufacturing, computer models alone are of limited use. When combined with advanced experimental methods, however, new opportunities arise. For example, models can be used to interpret experimental results in more detail, or to transfer experimental data obtained in the laboratory under ideal conditions to commercial production.

The method developed by Hocker and his team starts by measuring inline temperature and heat flux to characterise chocolate crystallisation under real production conditions. The next step is to use differential scanning calorimetry (DSC) tests to predict chocolate crystallisation under ideal conditions, before using these models to predict the crystallisation behaviour under real manufacturing conditions in the cooling tunnel.

Because these are new approaches in chocolate R&D, the team had to overcome several hurdles. For example, they developed new hardware to make precise temperature and heat flux measurements using specially prepared chocolate moulds that were deployed in the production line at Felchlin. In addition, they scrutinised established measurement procedures for characterising chocolate samples using lab equipment – such as DSC tests, Shukoff flasks and tempermeters – and developed and tested new procedures.

> A [research] collaboration has developed computational models to predict the crystallisation of chocolate and improve the commercial chocolate manufacturing process

IMPACT ON COMMERCIAL MANUFACTURING

Some chocolate manufacturers do not have their own R&D groups. Such companies need simple, robust tools that can be used with little experience, such as the newly developed hardware tools to make accurate temperature measurements during the production process and software tools to analyse the obtained data. Meanwhile, larger chocolate manufacturers with existing laboratory testing facilities could benefit from more sophisticated modelling that requires laboratory test results for input parameters. This could include using DSC data to characterise the crystallisation of chocolate under laboratory conditions and the subsequent use of models to predict crystallisation in the production line.

As Hocker explains, the methods his group has devised have several advantages. "For instance, we have the ability to assess the impact of changes in equipment and operating conditions, allowing us to evaluate the impact of these changes on optimised product quality, speed up the integration of new equipment into the production process and quickly adjust process parameters to new chocolate products," he says.

Hocker's newly developed methods have yet to be fully implemented in the day-to-day processes of his chocolate manufacturing partners. Each company is unique, with diverse product ranges and specific needs. Thus this forward-thinking Swiss collaboration is currently planning a follow-up project to establish a number of different workflows tailored to the different needs of each chocolate manufacturing company. The hope is that this will eventually result in the production of even better chocolate.