Chocolate physics: How modeling could improve 'mouthfeel'

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Chocolate. Credit: Wikimedia Commons

Lecithin is an ingredient that you've probably never heard of, but one that plays a vital role in the production of chocolate and many other foods. It's never been clear how this ingredient works on a molecular level, and confectioners have relied on observational methods - essentially trial and error - to perfect their recipes.

Now, scientists have shown how the field of molecular dynamics (simulation on a molecular level) could be a valuable tool in understanding chocolate conching - the part of the chocolate-making process where aromatic sensation, texture and 'mouthfeel' are developed.

Writing today in the *Journal of Physics D: Applied Physics*, the researchers, based at Technische Universität München, Germany, report

that they were able to use molecular dynamics to gain new insights into the molecular interactions during chocolate conching.

"There are many hypotheses on how lecithins work during the manufacturing of chocolate," explains Heiko Briesen, a lead author on the paper. "But we've been able to shed some light on the mechanism of this process."

Asking the right question was the important first step according to Briesen. "Molecular dynamics only allows us to model scales of nanoseconds or nanometres - and this process happens in minutes or hours in reality."

"But when we ask a specific enough question - like how does the lecithin molecule attach to the sugar surface - it can become incredibly powerful."

Understanding this mechanism is a key question for food chemists, as the commonly used lecithin is sourced from soy beans, but a decreasing supply of non-genetically modified (GM) soy beans means that sourcing non-GM lecithin is increasing difficult. Without a way of simulating how different lecithins will affect the chocolate-making process they are reliant on trial-and-error.

"I'm quite confident molecular dynamics will strongly support food science in the future" concludes Briesen.

More information: "Interactions between phospholipid head groups and a sucrose crystal surface at the cocoa butter interface" *Journal of Physics D: Applied Physics*, 48 384002. iopscience.iop.org/0022-3727/48/38/384002/article

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