EXPLORING MOLECULAR COLLISIONS

Professor Hanna Vehkamäki applies quantum chemistry and computer simulations to reveal the mechanism behind molecular clustering. The collisions of the nano-sized particles play a key role in climate regulation

The grants appropriated by the European Research Council are not easy to acquire. Thousands of competent scientists apply for them every year, and usually a research group is granted only once. Physicist Hanna Vehkamäki is one of the very few scientists who has received an ERC grant twice. A few weeks ago she was awarded a sum of €2.4m to study aerosol and ice crystal formation in the atmosphere. Vehkamäki and her group are going to explore the collisions of the nano-sized clusters by using advanced computational methods of quantum chemistry and physics. They are powerful new tools in atmospheric sciences.

Scientists around the world have been working for decades to find out the origin of the so-called 'secondary aerosol particles'. This has been Vehkamäki's field, too. The tiny particles suspended in air are borne in Nature: for example, boreal forests emit gaseous chemical compounds which can, after a few complex microphysical processes, form aerosols and grow up to sizes where they can act as cloud droplet seeds. Thus aerosols not only affect visibility and human health, but they also regulate the climate in many ways.

"The formation process of the aerosols is known by and large quite well, but what actually happens at the molecular level is not clear. This might sound like a detail, but as long as we do not know the primary driver of clustering, we cannot predict the climate either," explains Vehkamäki.

To stick or not to stick?

During clustering, molecules collide with each other, after which they either stick together or break up back into separate parts.

Hanna Vehkamäki, professor of computational aerosol physics at the University of Helsinki

Processes like this are extremely difficult to study experimentally. First, the clusters are less than a nanometre in diameter, and thus most instruments do not detect them. Second, the smallest clusters may not be stable and can be affected by the measurement itself, which distorts the results. This is why Vehkamäki and her group now use a wide palette of methods including simulations and computational fluid dynamics.

"Computer modelling is an extremely powerful tool in modern science, but simulations can by no means substitute the laboratory experiments performed with, say, mass spectrometers. On the contrary, experiments, computer modelling and theoretical analysis complement each other."

As a byproduct of their work, Vehkamäki's group might later develop commercial applications in the area of atmospheric technology and programming. "But it is not the aim," Vehkamäki emphasises. She is not motivated by climatics either. "Atmospheric problems are, of course, interesting and important from the point of view of humankind. But personally I am most fascinated by the molecules and their behaviour. I simply want to know the fundamental laws governing the Universe."

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