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Towards a molecular-based parameterization of the ice nucleation activity of biological macromolecules and its implications for aerosol-cloud interactions

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Primary biological aerosol particles (PBAPs) play an important role in mixed-phase clouds as they nucleate ice even at temperatures of $T > -10$ °C. Current parameterizations of PBAP ice nucleation are based on ice nucleation active surface site (INAS) densities that are derived from freezing experiments. However, only a small fraction of the PBAP surface is responsible for their ice nucleation activity, such as proteins of bacteria cells, fungal spores, pollen polysaccharides and other (unidentified) macromolecules. Based on literature data, we refine the INAS density parameterizations by further parameters:

- 1) We demonstrate that the ice nucleation activity of such individual macromolecules is much higher than that of PBAPs. It can be shown that INAS of PBAPs can be scaled by the surface fraction of these ice-nucleating molecules.
- 2) Previous studies suggested that ice nucleation activity tends to be higher for larger macromolecules and their aggregates. We show that these trends hold true for various groups of macromolecules that comprise PBAPs.

Based on these trends, we suggest a more refined parameterization for ice-nucleating macromolecules in different types of PBAPs and even for different species of bacteria, fungi, and pollen. This new parameterization can be considered a step towards a molecular-based approach to predict the ice nucleation activity of the macromolecules in PBAPs based on their biological and chemical properties.

We implement both the traditional INAS parameterization for complete PBAPs and our parameterization for individual molecules in an adiabatic cloud parcel model. The extent will be discussed to which the two parameterizations result in different cloud properties of mixed-phase clouds.