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A practical resource for common modelling approaches in simulating planetary volatiles

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The modelling of planetary volatiles is inherently interdisciplinary, encompassing a wide range of physical processes that operate across vastly different spatial and temporal scales. Despite the increasing importance of volatiles for understanding planetary evolution, surface–exosphere interactions, and resource potential, the existing literature remains highly specialised and fragmented. This presents a significant barrier to entry for researchers and early-career scientists seeking to engage in this field. In response to this challenge, we present a new book project that provides a comprehensive, accessible, and integrative overview of modelling approaches used in planetary volatile studies. The book is currently being prepared for publication with Elsevier in 2028.

At the most fundamental level, volatile-surface interaction is governed by atomic- and molecular-scale processes. These include adsorption, desorption, diffusion, and chemical reactions, which are typically investigated using techniques such as Density Functional Theory and Molecular Dynamics. Modelling on this atomic scale provides insights into binding mechanisms, reaction pathways, and kinetic processes that determine volatile stability and mobility. At the grain scale, particle–surface interactions, as well as heat and mass transfer processes, dominate volatile behaviour. Modelling approaches account for the heterogeneous nature of regolith grains, including surface chemistry, morphology, size distribution, and porosity. Heat and mass transport models are essential to capture the exchange of volatiles between the subsurface and the surface, especially under diurnal temperature variations characteristic of airless bodies. At the macro scale, the composition of exospheres and the migration of volatiles are commonly modelled using Monte Carlo methods to track particles originating from release processes via surface interactions, while accounting for surface temperature distributions and topography.

The presented book provides a structured introduction to commonly used computational and theoretical methods, highlighting their assumptions, limitations, and domains of applicability. In addition to theoretical foundations, the book follows a handbook approach, with practical guides, methodological comparisons, illustrative use cases and exercises. By synthesising methodologies from different fields of research into a unified resource, it aims to lower the barrier to entry for new researchers while also serving as a reference for experienced practitioners. Ultimately, this book aims to provide a foundation for future advances in the study of volatiles and their role in shaping planetary surfaces and environments.