Clouds in Exoplanetary Atmospheres

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1 Introduction

Today, we know 4330 exoplanets orbiting their host stars in 3200 planetary systems\(^1\). The diversity of these exoplanets is huge, and none of the known exoplanets is a twin to any of the solar system planets, nor is any of the known extrasolar planetary systems a twin of the solar system. Such diversity on many scales and structural levels requires fundamental theoretical approaches. Large efforts are underway to develop fundamental theoretical approaches for individual aspects of exoplanet sciences, like exoplanet atmospheres, cloud formation, disk chemistry, planet system dynamics, mantle convection, mass loss of planetary atmospheres.

The diversity of exoplanets calls for a fundamental, for an interdisciplinary and for an intelligent approach in order to fully understand their atmospheric composition. Many harbour a dynamic atmosphere where cloud particles can form in abundance. Some planets will be fully covered in clouds, some have clouds on the nightside but are largely cloud-free on the dayside. The basic processes of cloud formation are understood, and the main challenge lays in the fundamental physics and chemistry of material properties. The simultaneous development of different cloud models (e.g., \([14, 21]\) has enabled great insight into individual processes which now need to be combined. Such a combination requires an intelligent approach for tackling the micro-physical complexity involved. This includes the modelling of cluster formation, particle-particle growth/destruction, ionisation and photo-processes, diffusion and turbulent transport consistently coupled. Cloud models are a key part of the virtual laboratories that enable us to study the large parameter range of exoplanets, and to decipher the combination of individual observations.

Several of the known exoplanets orbit their host star very closely such that a rocky surface turns into magma ocean (e.g. CoRot-7b or 55 Cnc e) or Jupiter-like exoplanets expand their atmosphere considerably (e.g. HD 189733b, HD 209456b) and asymmetrically (e.g. HAT-P-7b, WASP-18b). Inside the atmospheres of exoplanets, clouds form. The cloud particles (aerosols) are made of a mix of minerals, for example, silicates and iron oxide in giant gas planets \([15]\), and sulfur hazes \([8]\). The global cloud composition changes with changing element abundance which can be affected by outgasing (e.g. for 55 Cnc e; \([25]\)) and pre-determined by the location of planet formation within the disk \([18, 12, 9]\). The composition of the upper crust of a rocky planet does determine the atmospheric element abundances, and eventually, the stability of liquid water \([18]\).

Hydrocarbon hazes have been shown to form in the upper atmospheres of super-Earths and mini-Neptunes (e.g. GJ 1214b and GJ436b; \([20]\)) under the effect of the UV radiation field of the M-dwarf type host stars. Similar effects have been proposed for the day-side of the giant gas planet WASP-43b where the UV photons of a K star enable the formation of hydrocarbon hazes in tandem with mineral cloud particles \([12]\). Spectroscopic studies of exoplanets are repeatedly frustrated by clouds and/or hazes blocking the view into the underlying atmosphere to reveal the existence of potential biosignatures, signature for their evolutionary state, or traces of planet formation. Clouds on Earth are linked to the support of the terrestrial cycle of life as they can preserve the right temperature of the biosphere and enable the transport of water through the atmosphere. Cary exoplanet clouds as similar significance?

The following challenges need to be addressed in order to answer this question, and, simultaneously provide the opportunity to progress our understanding of exoplanets and their atmospheres by exploring our

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models as virtual laboratories to fill gaps in observational data from different instruments and missions, and taken at different instances of times:

Challenge a) Building complex models based on theoretical rigor that aim to understand the interactions of atmospheric processes, to treat cloud formation and its feedback onto the gas-phase chemistry and the energy budget of the planetary atmosphere moving away from solar-system inspired parameterisations.

Challenge b) Enabling Cloud modelling based on fundamental physio-chemical insights in order to be applicable to the large and unexplored chemical, radiative and thermodynamical parameter range of exoplanets in the universe. Challenge b) will be explored in what follows.

2 State of the art - Cloud formation modelling

The results of atmosphere models [6, 19, 38, 35, 5, 26, 3, 22, 27], or retrieval approaches [24, 1, 2, 28], will depend on their individual components, their ability to model physics and chemistry and to solve it numerically. Cloud formation modelling in Earth and solar system atmosphere modelling, e.g. [34, 17], has a long tradition. It is essential that different modelling approaches are followed in order to enable a benchmarking process. Cloud formation modelling is also a key component in atmosphere modelling and retrieval for exoplanets where the atmospheric gas is chemically and dynamically very different to what is known from our solar system. Cloud particles are tracers of the gas from which they form, through which they move, which they deplete or enrich with respect to elements abundances, and which they heat or cool due their opacity. In order to understand the chemical composition of exoplanet atmosphere, to link this composition to their evolutionary state by interpreting observations from CHEOPS, HST, JWST, Ariel, PLATO etc., cloud formation needs to be understood in enough detail to be applicable to the diversity of known exoplanets. Such a cloud model needs to be applicable to the wide ranges of thermodynamics, radiation and chemical regimes that exoplanets have presented us with. Here we lay out the challenge of building such a cloud model, starting from our kinetic modelling philosophy. This is not a speedy exercise and retrieval modeller may therefore still wish to hold on to representing a cloud by a set of parameters like particle size, or by reducing complexity by keeping physical consistency [29].

2.1 Basic processes to form a cloud particle

Seed formation: Unless an exoplanet has dust particles or other condensation seeds swapped into its atmosphere (e.g. condensing meteoritic dust, volcano outbreaks, sand storms), the formation of a cloud particles begins in the gas phase by chemical reactions of those atoms/molecules/ions that are available in the atmosphere of a certain element composition. The element composition and the local thermodynamic conditions determine the first condensates. The formation of condensation seeds can be understood as a chain of chemical gas-gas reactions that progresses to molecules and clusters with increasing size and complexity. The challenge is to determine the required thermodynamic cluster data, the free energy change associated with the formation of a cluster of size \( N \), \( \Delta G(N) \). Assuming that no activation energy is required, one can formulate a rate network for all cluster sizes [30] or approximate \( \Delta G(N) \) based on the concepts of classical nucleation theory [23]. If cluster formation requires an activation energy, all individual chemical reaction will need consideration. Such fundamental concepts enable the modelling of the formation of mineral and organic seeds for a wide range of chemical situations if the required material data (e.g. \( \Delta G(N) \)) are available. Further chemical paths open up in highly irradiated planets where photochemistry leads to the formation of hydrocarbon molecules of increasing complexity after carbon is released by photochemically destroying CO or \( \text{CH}_4 \) [21, 33]. Two chemically independent ensembles of seed particles maybe expected in highly irradiated exoplanets, as shown for WASP-43b [12]. It needs to be understood, however, that a seed formation rate will depend on how much elements are consumed by further bulk growth.

Bulk growths: Once seed particles are present, the gas phase can easily condense on these surfaces because non-photochemicaly-driven seed formation requires a supercooling of the gas phase which is then highly supersaturated. The kinetic bulk growth of cloud particles of mixed composition by gas-surface reactions can efficiently be modelled through a moment method that provides consistent information about cloud particle composition, particles sizes and cloud extension [14]. A challenge are the details of the 100’s surface
Figure 1: The exoplanet atmosphere challenge: Ultra-hot Jupiters combine an ultra-hot dayside forming an ionosphere with a high degree of ionisation (thermal degree of ionisation, \( f_e \) – blue-yellow-red colour coded) with a cloudy nightside (\( \rho_d/\rho_{\text{gas}} \) - black surface contour lines), shown here for HAT-P-7b as slice plot through the equatorial plane. The atmospheric pressure levels are shown as concentric rings [courtesy to D. Samra].
reactions which remain largely unexplored by laboratory studied. A further process of increasing particles
sizes is coagulation, i.e. the collisional growth of existing cloud particles. This can occur for hydrocarbon
monomers or for mineral cloud particles if the relative velocities are appropriate. Collisions between cloud
particles may also lead to shattering causing a decrease of the mean particle size but an increase in particles
number [10]. The arising challenge is that binning methods work well for solving Smolochovsky’s coagulation
equation in a mass conserving scheme but are challenged by particles of mixed materials. Modelling the
kinetic surface growth and the collisional growth of existing dust particles furthermore requires to determine
the cloud particle velocity in potentially different frictional regimes.

Gravitational settling, frictional coupling, turbulent mixing and diffusion: Cloud particles move. Frictional coupling of cloud particles to the gas phase determine how far cloud particles of certain sizes and
masses fall into the deeper atmospheric layers (and hence, keep growing or begin to evaporate). They
stand still (relative to the surrounding gas) in the gas of complete friction (i.e. position) coupling with the
gas. Frictional coupling does also determine in how far turbulent gas motion affects their further growth
or even their ionisation. In case of complete coupling, turbulence will cause the formation of intermittent
cloud structures due to the emergence of vorticity [13]. Diffusion is often used as overarching term for
transport against the atmospheric pressure gradient and turbulent mixing as a driver of such diffusion. Per
definition, diffusion is driven by concentration gradients of gas-species but also of cloud particles. Each cloud
particle size would diffuse differently. Incorporating cloud particle diffusion in cloud models has proven to
be challenging, not the least because cloud particle diffusion coefficients are unknown [40].

Neutral gas-phase chemistry: Modelling cloud formation requires knowledge about the local thermo-
dynamic conditions, including the chemical composition for a set of element abundances. This, in turn,
will depend on the presence of a condensed phase [18]. The most complete set of information about the
gas-phase composition for almost all elements that we know from the Sun’s atmosphere (incl. O, Mg, Fe,
Si, Ca, Na, Al, Ti, ...) is provided by chemical equilibrium calculations (e.g. [39]). Large gas-kinetic or
photochemical calculations remain limited to molecules made of C/H/N/O and S and can, because of their
complexity, be complete only unto a certain number of elements per molecule [32]. C/H/N/O are used to
study the formation of hydrocarbon hazes and the triggering of possibly biology related molecules like HCN.
Such constrained chemical networks are very efficient for the study of specific processes, like for example,
lightning chemistry [32] and biomolecules on the surface of charged cloud particles [37]. The challenge is far
more fundamental, namely, to build kinetic rate networks that link to the need of the nucleation modelling
outlines above and to model spectacular events like lightning in the exoplanet context.

2.2 Ionisation process

Atmospheres of exoplanets can be highly irradiated such that the atmospheric gas is photoionised and/or
ionised thermally. The ionisation efficiency may vary from day to night side leading to a highly ionised and
cloud-free dayside and a cloudy nightside with just an ionosphere ontop on hot rocky planets like 55 Cnc e
[25] as on super-hot Jupiters [11]. The photoionisation can reach the upper cloud layers, but a more realistic
process is that currents from the ionised atmosphere form and transport charges onto the surface of the
cloud particles, similar to Earth.

Figure [1] demonstrate that for the ultra-hot Jupiter HAT-P7b the day/night difference of the thermal
degree of ionisation (colour coded). An ionosphere is extending deep into the dayside atmosphere but remains
rather shallow on the nightside. The nightside, in contrast is covered in clouds (solid black lines show the
cloud-particle mass loss in term of the dust-to-gas mass density ratio) which also assymetrically cover the
two terminator regions.

3 Opportunities

Understanding if the atmosphere of an exoplanet enables biological activity requires us to understand the
interaction of every-day processes that occur on Earth in a far larger parameter range than available on
Earth. This is why laboratory experiments on Earth are unfortunately only of limited value for exoplanet
research in its whole diversity of exoplanet species. The exoplanet parameter range is increased by being linked to the evolutionary state of the planet, and its formation history. We therefore require complex models to study in detail the physico-chemistry of exoplanet atmospheres, what is more, we require several of those models to be developed in parallel to be able to follow the fundamental research ethics of testing and comparing results by different means and apertures. The use of only one model defeats the purpose of research and the necessary falsification of results.

Building virtual laboratories by virtue of complex models is the only path to understand the vast exoplanet diversity in depth, and to decode observations that can only be taken for selected times (or time intervals) and for selected wavelengths (or wavelength bands) for selected objects. Monitoring exoplanets of different kinds, that orbit different stellar types, in wavelengths and in time is unfeasible in the foreseeable future. The purpose of such monitoring could be as far-fetched as finding a proper landing side or as fundamental as understanding the different planets as global objects. The EAS Voyage 2050 white papers on exoplanet research remain focused by necessity, including spectropolarimetry [7], spatial resolved mid-IR of thermal emission [31] and high-contrast imaging [36] missions as next steps beyond JWST, Ariel and the ELT-class telescopes. Modelling the underpinning exoplanet atmosphere physics and chemistry will be essential. Virtual laboratories already enables us to explore exoplanet atmosphere with respect to specific processes (like the effect of cloud formation), or as the sum of all known processes (like the emerging of weather pattern), and in particular beyond the singled-out terrestrial conditions (e.g. for a diversity of element abundances).

4 Challenges

Outstanding Challenges to enable virtual laboratories to meet the observational challenge include:

- the element abundances that determine the planet’s atmosphere chemistry
- chemical and cluster data for all possible nucleation species
- thermochemical data for reaction rates for element other than C/N/O/H/(S)
- thermochemical data for gas-surface reactions, incl. sticking probabilities
- opacity data for condensates across large wavelengths ranges and crystalline species
- opacity modelling for non-spherical and charged cloud particles.

Meeting these challenges will enable us to decipher the evolutionary state and the planet’s formation mechanisms spectroscopically, and to determine with confidence the state of habitability of an extrasolar planet.

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