From Organic Materials to Metal Powders: Moisture Adsorption and Water Vapour Equilibrium Points

In this white paper, Relequa's founder Dr Peter Moir delivers the first detailed, practical explanation of the Water Vapour Equilibrium Point (WVEP) — linking its thermodynamic foundation to real-world kinetic behaviour — and shows how this insight transforms our understanding of moisture in both organic materials and metal powders.

Introduction

The behaviour of water in materials, whether food products, pharmaceuticals or metal powders, is governed by the concept of water activity – a measure of the escaping tendency of water from a material relative to that of pure water at the same temperature. Water activity, denoted a_w, is defined thermodynamically as the ratio of the vapour pressure of water in the material to the vapour pressure of pure water. It reflects the chemical potential of water in the material; lower water activity corresponds to more "bound" water and a lower chemical potential, meaning less tendency for water molecules to leave the material. Water activity has profound implications for microbial growth, stability of active ingredients and shelf life. Recent techniques such as Relequa's moisture profiling define a Water Vapour Equilibrium Point (WVEP) as the relative humidity at which a material's moisture profile stabilises – the humidity at which the rates of water adsorption and desorption become equal (1). The WVEP provides a macroscopic fingerprint of how strongly a material binds water. Understanding the microscopic processes that give rise to the WVEP, and how these processes differ between organic materials and metal powders, requires linking concepts from thermodynamics, surface chemistry and molecular dynamics.

This article begins by explaining water activity and the thermodynamic driving forces behind moisture adsorption and desorption in organic materials. It then shows how the balance of chemical potentials leads to a WVEP that is characteristic of a material's surface chemistry. Building on this foundation, the article surveys the growing body of molecular-level studies on water interacting with metal surfaces and metal–oxide powders. By comparing the dynamics of water adsorption on organic and inorganic materials, we highlight both universal aspects of interfacial water and the distinctive phenomena that arise from metallic bonding and oxide chemistry. The article concludes with an overall summary and perspectives on future research.

Water Activity and the Continuum of Bound and Free Water in Organic Materials

When we talk about water in a material, it is tempting to classify it as either "free" or "bound." In reality there is a continuum of binding energies. Water molecules form hydrogen bonds with polar functional groups, pack into capillaries, solvate ions or remain in loosely associated pools. The water activity concept formalises this continuum: it quantifies how tightly water is held by reporting the ratio of the vapour pressure of water in the material to that of pure water at the same temperature. A water activity of 0.70 means the vapour pressure is 70% of that above pure water; the chemical potential of water in the material is correspondingly lower. A widely cited guideline emphasises that even "strongly bound" water is not immobilised; water activity measures how tightly water is bound and relates to the work required to remove it (2). In other words, bound water still participates in dynamic exchange with the vapour phase – it simply has a lower escaping tendency.

The chemical potential μ_w of water in a material is related to water activity by

$$\mu_w = \mu_w^0 + RT \ln a_w$$

where R is the gas constant, T the absolute temperature and μ_w^0 the chemical potential of pure water. When a material is exposed to air of a given relative humidity (RH), the system tends toward equilibrium when the chemical potential of water in the material equals that in the surrounding air. If the relative humidity of the environment is higher than the material's water activity, water will be adsorbed until the activities equalise; if it is lower, water will desorb. Thus, the direction of moisture transfer is driven by chemical potential gradients, not simply by whether the water is "free" or "bound."

Molecular-Level Mechanisms of Moisture Adsorption/Desorption in Organic Materials

At the microscopic level, water adsorption and desorption involve collisions between gas-phase water molecules and the material surface. Molecular-beam experiments provide some of the most detailed insights into these processes. For example, when hyperthermal water molecules (~0.29 eV) were directed at condensed *n*-butanol surfaces, only a small fraction scattered back into the gas phase. The majority became trapped on the surface; the trapped molecules were released via two regimes of desorption: a fast regime with residence times shorter than 10 μs and a slower regime lasting 0.8–2 ms (3). This study showed that water molecules lose between 60 % and 90 % of their incident kinetic energy on impact and typically retain only 10–40 % of their initial energy upon scattering. The energy dissipation channels include excitation of lattice vibrations (phonons), electron–hole pair creation and conversion of translational energy into rotational or vibrational modes of the water molecule (4).

Once water is adsorbed, its excess energy must be dissipated. On organic surfaces, dissipation is dominated by the hydrogen-bond network. Pump–probe experiments that

resonantly excited intermolecular modes of liquid water found that energy deposited into rotational motion is transferred to translational motion of neighbouring molecules on a time scale of ~0.5–0.75 ps (5). Molecular-dynamics simulations show that the translational kinetic energy of an excited water molecule peaks around 0.2 ps and relaxes back to equilibrium within 0.5–0.75 ps. These ultrafast energy-transfer processes explain why water is such an efficient heat sink and why moisture adsorption events do not generate measurable temperature changes under typical conditions.

The micro-kinetic picture reveals that even strongly bound water molecules desorb on microsecond to millisecond time scales (6). In a macroscopic experiment, however, millions of such adsorption/desorption events occur per second across the huge surface area of the material. At the WVEP – the relative humidity at which the material's headspace humidity stabilises – the net flux of water becomes zero because the adsorption and desorption rates are equal. This dynamic equilibrium is achieved without a temperature increase because each desorption event is compensated by an adsorption event, and the latent heat released on adsorption balances the enthalpy required for desorption. Materials with a low WVEP (e.g., hygroscopic powders that reach equilibrium at 35% RH) often take hours to equilibrate (1) because their binding sites have relatively high activation energies for desorption (3); however, on the scale of individual molecules the desorption events themselves are extremely rapid.

Water Vapour Equilibrium Point (WVEP) and Surface Chemistry

The WVEP is intimately linked to a material's surface chemistry. Materials rich in hydrophilic functional groups (e.g., hydroxyl, carboxyl, amino groups) form strong hydrogen bonds with water. When a water molecule adsorbs, it moves from a higher-energy gas phase to a lower-energy adsorbed state; the difference in chemical potential is dissipated via lattice vibrations and reorganisation of the hydrogen-bond network. Because these sites provide strong binding, only a relatively low vapour pressure is needed to saturate them; the WVEP is therefore low. Conversely, materials with hydrophobic surfaces (e.g., waxes or nonpolar polymers) have weak interactions with water. Water molecules tend to bounce off or remain loosely bound, retaining a significant fraction of their kinetic energy. As a result, equilibrium is reached only at higher relative humidities, and the WVEP is high.

An illustrative way to think about the WVEP is in terms of sorption isotherms. Sorption experiments measure how much water a material adsorbs at different relative humidities. At low RH, strongly binding sites fill rapidly. As RH increases, additional layers form or water enters capillaries and pores. The sorption curve often exhibits a sigmoidal shape; the steepest region corresponds to the point where multilayer adsorption or capillary condensation begins. The WVEP corresponds to the relative humidity at which the sorption curve crosses the material's internal water activity. This is the point where the chemical potential of water in the material equals that of the surrounding vapour, so there is no net uptake or release of moisture.

Because the WVEP is defined by chemical potential, it depends primarily on the strength and availability of surface binding sites rather than the absolute amount of free water. However, WVEP is not independent of the overall moisture content; as a material takes up more moisture the proportion of weakly bound water increases and the equilibrium relative humidity rises, and as it dries the WVEP falls. This is why in moisture profiling the WVEP value increases with moisture uptake and decreases as moisture is lost. In contrast, water that is tightly incorporated into a crystal lattice (so-called water of crystallisation) contributes little to the WVEP because it has no escaping tendency unless the crystal structure is disrupted. Overall, WVEP reflects both the strength and number of accessible binding sites and the current distribution of moisture among those sites. Materials with abundant strongly binding sites (e.g., hygroscopic powders or amorphous polymers) exhibit low WVEP values and take longer to reach equilibrium because water molecules must diffuse into the bulk to find unoccupied sites. Materials with predominantly weak binding sites (e.g., hydrophobic powders or crystalline sugars) have higher WVEP values and equilibrate quickly because water molecules desorb readily. Thus, the WVEP provides a macroscopic indicator of surface chemistry and moisture state.

What Is Known About Water and Energy Dissipation at Metal Surfaces?

Unlike organic solids, metal surfaces and metal oxides present a very different energy landscape to an incoming water molecule. Studies using density-functional theory and ab-initio molecular dynamics show that clean metal surfaces (Ag, Au, Pd and Pt, for example) are superhydrophilic; water spreads without forming a finite contact angle (7). The often-invoked “ice-like bilayer” model of water on metals has been superseded by an evolving picture in which adlayer molecules rearrange dynamically and interact strongly with the metal through electronic polarisation. On noble metals the first water layer binds with energies around 0.5 eV per molecule – similar to strong hydrogen bonds in ice – and can rearrange without a high energy penalty.

More complex behaviour on metal-oxide surfaces

Most metal powders do not present bare metal surfaces; instead, they are covered by native oxide layers. The chemistry of these oxides strongly influences water adsorption. A recent computational study used DFT and ab-initio molecular dynamics to compare water adsorption onTiO_2, RuO_2 and IrO_2 showed that adsorption energies increase from TiO_2 to IrO_2 and that the stability of molecular versus dissociative adsorption depends on surface orientation and water coverage (8). RuO_2 and especially IrO_2 favour dissociative adsorption (formation of surface hydroxyls), because the d-bands of the heavier metals accommodate the charge transfer associated with OH formation more readily than TiO_2 does. This implies that on some oxides water binds by forming hydroxyl groups rather than remaining intact.

Calculations also reveal cooperative effects. The adsorption energy of water depends on the number and arrangement of neighbouring molecules: hydrogen-bond networks can stabilise or destabilise the adsorbed species. For example, adding a second water molecule can stabilise the dissociative state on TiO_2 by facilitating proton transfer, whereas on IrO_2

additional water can destabilise the intact molecular state by crowding the surface . Thus, the structure of the interfacial water layer depends sensitively on both the metal oxide and the local water coverage. For metal powders, this means that factors such as oxide thickness, crystallographic orientation and humidity will determine whether water remains molecular or dissociates to hydroxyls.

Bimetallic surfaces add another level of complexity

The composition of a metal surface can strongly modify its interaction with water. Density-functional theory studies on bimetallic Pt–Ru alloys show that Ru atoms bind water more strongly than Pt atoms. One ab-initio MD study of a PtRu/Pt(111) alloy found that even at room temperature water molecules preferentially occupy Ru sites, and the water–Ru binding energy is higher than that on Pt (9). Such findings are relevant for electrocatalysts, where the local arrangement of atoms can affect the structure of the hydration shell and thereby influence reaction rates.

Comparison of Organic Materials and Metal Powders Binding Energies and Surface Interactions

Organic materials generally interact with water through hydrogen bonding and van der Waals forces. The binding energies range from a few tens of kilojoules per mole for primary adsorption sites to a few kilojoules per mole for multilayer adsorption. The n-butanol molecular-beam experiments indicated desorption activation energies of 27–37 kJ mol^{-1} (2). In contrast, water adsorption on metal surfaces involves stronger interactions. DFT calculations yield binding energies of ~0.5 eV (~50 kJ mol^{-1}) per water molecule for the first layer on noble metals. On metal oxides, dissociative adsorption can form OH groups with bond energies exceeding 400 kJ mol^{-1}. These strong interactions imply that water molecules may not simply physisorb but can chemisorb or dissociate on metal surfaces, altering the surface chemistry.

Surface Structure and Dynamics

On hydrophilic organic surfaces, water molecules form hydrogen-bond networks similar to those in bulk water. The dynamic reorganisation of these networks occurs on picosecond time scales. On clean metal surfaces, water forms strongly bound adlayers with negligible contact angles. These layers can be more ordered or even exhibit lattice matching to the underlying metal. On metal oxide surfaces, the presence of surface hydroxyls or defects can lead to a mixture of molecular and dissociative adsorption states.

Kinetics and Equilibrium

In organic materials, water molecules continually adsorb and desorb, reaching dynamic equilibrium at the WVEP. Residence times on the order of microseconds to milliseconds mean that even strongly bound water is mobile. The WVEP reflects the humidity at which the average chemical potential of water in the material equals that of the surrounding

vapour; it is determined by the density and strength of binding sites. For metal powders, the concept of water activity and WVEP is less commonly applied, but the same thermodynamic principles hold. Because water binds strongly to metal surfaces, the "equilibrium relative humidity" required to achieve a given water coverage may be much lower than in organic materials. However, this equilibrium may not correspond to simple physisorption but to a state with chemisorbed hydroxyls or dissociated water. Moreover, metal surfaces can undergo slow structural changes (e.g., oxidation, corrosion) when exposed to water, so equilibrium may involve transformations beyond adsorption/desorption.

Moisture Uptake and Flowability of Metal Powders at High Humidity

While theoretical studies predict strong water binding on metal surfaces, relatively few experiments have directly measured moisture uptake and its consequences for metal powders. A notable example is the work of Cordova and colleagues (9), who investigated how typical laser-powder bed fusion (LPBF) feedstocks behave when exposed to humid, moderately warm environments. In their study four alloys—Inconel 718, Ti-6Al-4V, AlSi10Mg and Scalmalloy—were aged for 72 h in a climate chamber at 80% relative humidity and 50 °C to emulate the humidity and temperature inside a build chamber. This humid ageing was compared with vacuum drying (85 °C for 6 h), air drying (150 °C for 20 min) and the as-received state.

The alloys responded very differently to the humid treatment. Visual inspection after ageing revealed that the aluminium alloy AlSi10Mg developed a two-tone appearance: the upper layer was light grey while the lower layer remained darker, reminiscent of wet beach sand. This suggests that moisture penetrated unevenly through the powder bed. All four powders exhibited some degree of particle agglomeration after humidity exposure, although in most cases the agglomerates could be dispersed by gentle shaking. In contrast, scanning electron microscopy showed no detectable changes in particle morphology due solely to moisture or drying treatments.

To quantify moisture uptake, the authors measured the mass loss upon drying using a moisture analyser. The AlSi10Mg powder absorbed the most water during the 72-h, 80% RH ageing. Inconel 718 and Ti-6Al-4V showed surprisingly little additional moisture; in fact, their air-dried samples sometimes retained slightly more moisture than the humid-aged samples, an effect attributed to experimental variability. Energy-dispersive X-ray spectroscopy (EDX) detected a small oxygen peak at 0.5 keV in moisturised AlSi10Mg that was absent in the as-received powder, indicating that some water remained bound as hydroxide or oxide on the particle surfaces.

The authors also examined how moisture affects flowability, a critical parameter for powder bed fusion. Using the ASTM Hall flowmeter, they recorded the time taken for 50 g of powder to flow through a standard orifice. Inconel 718 flowed the fastest under all conditions, while Ti-6Al-4V's flowability changed little after either drying or moisture uptake. By contrast, Scalmalloy and AlSi10Mg experienced severe flowability loss: vacuum drying improved their flow, but after humid ageing the powders were so cohesive that they would not flow through

the funnel at all. The researchers concluded that aluminium-based powders are far more sensitive to ambient humidity than their nickel- or titanium-based counterparts.

These findings have been echoed by subsequent studies. A 2024 investigation (10) of AlSi10Mg powder noted that moisture levels rise under conditions of high temperature and high humidity and fall under high temperature and low humidity; the authors cited Cordova et al.'s experiments at 80% RH and 50 °C for 72 h to support this trend. They also observed that high humidity promotes agglomeration by enabling weak bonding between satellite particles. Raman spectroscopy and SEM analyses confirmed that humid conditions favour the formation of aluminium oxides and hydroxides, although these surface films have only a minor effect on optical reflectivity. Together, these studies show that high humidity at elevated temperatures strongly affects aluminium-rich powders, increasing moisture uptake, inducing agglomeration and reducing flowability, whereas nickel- and titanium-based powders are more resistant.

Cordova's results can be interpreted in the thermodynamic framework established earlier. The powder surfaces are exposed to a fixed chemical potential of water corresponding to 80% RH at 50 °C. AlSi10Mg has a high affinity for water because of its oxide surface; once a monolayer of water forms, capillary condensation and the formation of hydroxide films further reduce the chemical potential, allowing additional water to adsorb. Inconel 718 and Ti-6Al-4V, on the other hand, have denser oxide films that limit water uptake. The observation that humid ageing had no measurable effect on powder temperature demonstrates that, as in organic materials, adsorption and desorption events are rapid and energy is dissipated efficiently. Unlike organic materials, however, water adsorption on metal powders can lead to chemical changes (e.g., oxide or hydroxide formation) and mechanical effects (agglomeration) that persist even after the humidity decreases.

Practical Implications

Understanding moisture adsorption on metal powders is critical for applications such as powder flowability, additive manufacturing, corrosion prevention and catalysis. Moisture can promote agglomeration, change surface charge, initiate corrosion or alter catalytic activity. The strong, often irreversible interactions between water and metal or oxide surfaces mean that powder handling under controlled humidity is essential. Reactive MD and DFT studies provide insights into these processes, but experimental data are needed to validate the predictions. Techniques such as environmental electron microscopy, infrared spectroscopy and temperature-programmed desorption could be employed to measure water adsorption states and kinetics on real powder surfaces.

Summary and Outlook

Water activity and the Water Vapour Equilibrium Point (WVEP) provide a framework for understanding moisture adsorption and desorption in organic materials. Water activity measures the chemical potential of water in a material; it reflects how tightly water is bound but does not imply that bound water is immobilised. At the WVEP, the chemical potential of

water in the material matches that of the surrounding vapour, so adsorption and desorption rates balance. Molecular-beam experiments on organic surfaces show that water molecules lose most of their kinetic energy upon impact and either scatter with reduced energy or adsorb and desorb on microsecond to millisecond time scales. Hydrogen-bond networks in water dissipate energy rapidly, leading to efficient thermalisation without macroscopic temperature changes. The WVEP reflects the density and strength of binding sites and therefore depends on surface chemistry.

The behaviour of water on metal powders is more complex but shares the same thermodynamic foundations. Computational studies reveal that clean metal surfaces are superhydrophilic and bind water extremely strongly. Metal oxide surfaces can further facilitate dissociative adsorption, forming hydroxyls and modifying the surface chemistry. Bimetallic surfaces can tune water binding energies, and reactive MD simulations show that hydration can restructure oxide surfaces and alter hydrogen-bond networks. While the concept of WVEP is not commonly applied to metal powders, one can think of an analogous equilibrium relative humidity at which a powder neither gains nor loses water. However, because water may chemisorb or dissociate, this equilibrium may be complicated by slow structural changes such as oxidation or corrosion.

Future research should aim to connect these molecular-level insights to macroscopic measurements. For organic materials, correlating sorption isotherms and WVEP values with microscopic binding energies could enable predictive models of shelf life and stability. For metal powders, experimental determination of water adsorption states and kinetics is essential. Combining techniques such as molecular-beam scattering, infrared spectroscopy, synchrotron X-ray scattering and reactive MD will be crucial to understand how humidity affects powder behaviour. Improved knowledge of water–metal interactions will impact fields ranging from additive manufacturing and catalysis to corrosion science and environmental geochemistry.

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