Estimating the hydratable surface area of building materials from water vapour sorption

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Abstract. The specific surface area of a building material controls its physical, chemical, and biological functions and services, including its moisture regulating potential. The Hydratable Specific Surface Area (H-SSA) of a building material can be estimated from its primary water vapour adsorption and desorption isotherm at a given relative humidity (RH) value or range of RH. The concept is illustrated for 12 mineral and bio-based building materials. The estimated H-SSA for only 1 kg of some building materials can approach the area of a typical agricultural field (500,000 m², 50 ha.), which helps explain and illustrate the great moisture regulating properties of many bio-based materials. The H-SSA appears useful to help characterize and classify building materials.

1. Introduction

Moisture regulation and mould prevention in buildings are heavily influenced by the water vapor sorption dynamics of building materials. The ability for water vapour uptake, storage and release, depend on the pore networks and active surfaces of the materials during adsorption and desorption, which occur during fluctuations in outdoor and indoor relative humidity. Despite the significance of understanding moisture behavior, the specific surface area (SSA) of building materials has rarely been measured.

The specific surface area (SSA) of building materials is a critical parameter that influences the Heat, Air, and Moisture (HAM) properties of materials, which in turn affects the indoor climate and energy consumption of buildings. Accurate measurement of SSA is essential for understanding and predicting the HAM properties of building materials. While various methods exist for measuring SSA, such as gas adsorption, mercury intrusion porosimetry, and BET analysis, they are often time-consuming and require expensive equipment. In this study, we propose an approach for estimating the SSA of a variety of building materials based on monolayer sorption from water vapour sorption isotherms. This method is simple, cost-effective, and can be applied to a wide range of materials.

This study takes inspiration from the field of soil physics, where a similar need for investigation of SSA can be found. In the determination of both soil- and building materials, there is a need for a simple yet reliable method. Concrete-based materials are an exception where surface area has been primarily quantified through nitrogen gas adsorption or theoretical particle size distribution methods [1,2]. However, these methods have limitations as nitrogen gas adsorption only measures external surfaces, and particle size distribution methods based on simple particle geometries tend to underestimate specific surface areas [2–4]. As a result, they are less relevant for building materials without well-defined particles, such as the emerging bio-based materials with complex and varying compositions including fibres of different lengths and shapes, and irregular internal pore networks. Thus, we suggest adopting a concept to estimate the hydratable specific surface area (H-SSA) using water vapor sorption isotherms, which is becoming a standard method for quantifying specific surface area within soil physics [5,6].

In the field of soil physics, SSA is determined by either the ad- or desorption isotherms at a given RH. However, there is no consensus on whether the adsorption (normally used) or desorption isotherm (rarely available) should be used. Theoretically, the desorption isotherm may be more accurate as it excludes limitations in water uptake caused by small and irregular pore systems, e.g., bottle-neck effect in the pores. Additionally, there is a debate on the RH at which SSA should be calculated, with 20-23% RH being the standard for non-expanding clay minerals and clay-rich soils [7], and 47% RH being suggested for expanding clay minerals [8]. Building materials often consist of a complex mixture of particles and fibres with both adsorption and desorption behaviour occurring frequently in the building envelope. Such behaviour depends on material compositions; mineral, hereunder silica-based, materials present different material-moisture interactions from bio-based materials, where water uptake occurs within cell walls [9], owing to their different pore structures, porosities and surface energies. Therefore, it may be more useful to introduce H-SSA as an interval rather than a single number to characterize and classify building materials. If a specific number is used, it should be clearly referenced to the applied RH and whether it is derived from adsorption or desorption.

Our aim is to introduce and demonstrate the H-SSA concept in building physics by analysing water vapor ad- and desorption isotherms for 12 different building materials, as studied in Frandsen et al. [under review]. These materials are selected to cover a diverse range of compositions. Furthermore, we seek to demonstrate how the H-SSA concept can be used to group building materials based on their moisture behaviour and other related physical, chemical, and biological processes influenced by their specific surface area.

2. Materials and Methods

2.1. Bio-based and Mineral Building Materials

Twelve building materials were investigated in this study. The materials can largely be categorized as either bio-based or mineral; they represent both different compositions and functions in building elements. Material acronyms, (dry) bulk densities and symbols are presented in Table 1.

Table 1 Overview of the twelve investigated building materials and their bulk densities at dry state.

	Material name			Bulk density [kg m^{-3}]
Bio-based	Pine wood	▲	PW	565
	Wood Fibre Insulation	■	WFI	50
	Eelgrass Insulation	◆	EGI	70
	Hemp Shives	●	HS	85
	Low-Hemp Hempcrete	◆	LH	445
	High-Hemp Hempcrete	■	HH	150
Mineral	Calcium Silicate	●	CS	225
	Unfired Clay Brick	◆	UCB	2022
	Aerated Autoclave Concrete	+	AAC	340
	Concrete	–	CON	2200
	Mineral Wool Insulation	+	MWI	29
	Ceramic Brick	×	BRI	1950

Water vapour sorption isotherms for all twelve building materials were generated in an existing study by Frandsen et al. [under review]. These were attained using the non-equilibrium Dynamic Dewpoint Isotherms (DDI) method applied in the fully-automated Vapor Sorption Analyzer (VSA), shown in Figure 1. Eight cyclic sorption isotherms were measured for each material with full ad- and desorption curves at 23°C, ranging from 10% to 90% RH with a resolution of ~4% RH. No pressure was induced on the materials during measurements. More information about the measurement campaign can be found in the study. Sorption isotherms (cycle 1) for each material are used in this investigation to estimate the SSA.

2.2. Calculating the Hydratable Specific Surface Area (H-SSA) by Water Vapour Sorption

Monolayer moisture content, also referred to as monolayer capacity, quantifies the mass of water molecules occupying the surface of a material in a single layer. It is intrinsically linked to the specific surface area (SSA) of a material, as this provides the area for water molecules to be sorbed onto. This relation is expressed by Equation 1.

$$SSA = (X_m \cdot N \cdot A) / M_W \quad (1)$$

SSA	Specific surface area [m^2 kg^{-1} material]
Xm	Monolayer moisture content [kg moisture kg^{-1} material]
N	Avogadro's number ($6.02 \cdot 10^{23}$ mol^{-1})
A	Surface area covered by a single water molecule ($10.8 \cdot 10^{-20}$ m^2)
Mw	Molecular weight of water (0.018 kg mol^{-1})

As Avogadro's number *N*, the surface area covered by a water molecule *A*, and the molecular weight of water M_w are physical constants, the specific surface area *SSA* has a linear relation to the monolayer moisture content X_m.

Figure 1. The Vapor Sorption Analyzer (VSA) used to measure water vapor sorption isotherms by the Dynamic Dewpoint Isotherms (DDI) method for the 12 building materials.

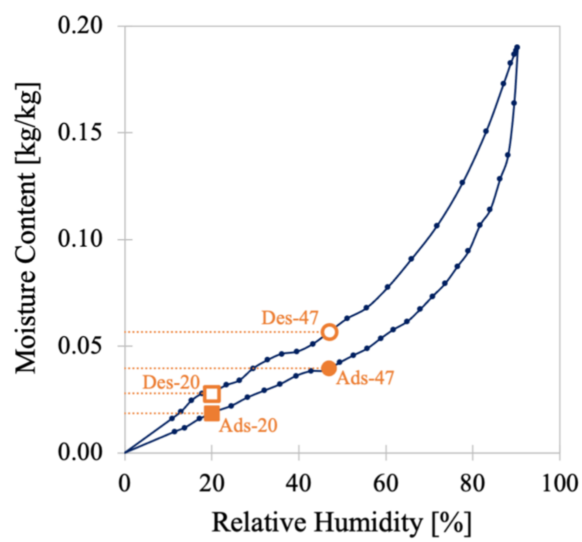

Figure 2. An example of moisture contents (Ads/Des; 20/47% RH) obtained from the water vapour sorption isotherm of High-Hemp hempcrete (HH).

In this study, the specific surface area (SSA) is defined as the hydratable SSA (H-SSA) to indicate that monolayer sorption occurs solely on hydratable pore surfaces, thereby excluding inaccessible closed pore surfaces. The monolayer moisture content is assumed to be achieved between 20% RH and 47% RH for all twelve building materials, and moisture contents are obtained at these relative humidities for both adsorption and desorption, as demonstrated in Figure 2. The range of moisture content at which monolayer moisture content occurs is defined as the monolayer interval. Utilizing Equation 1 on the water vapour sorption isotherms collected for the 12 building materials, the monolayer interval and subsequently the H-SSA can be evaluated using the four distinct moisture contents, namely Ads-20 (% RH), Ads-47, Des-20, and Des-47.

Moisture content is presented gravimetrically [kg moisture kg^{-1} material] and volumetrically [kg moisture m^3 material] in this study.

3. Results and discussion

3.1. Gravimetric Hydratable Specific Surface Area (H-SSA)

Figure 3 illustrates the gravimetric hydratable specific surface area (H-SSA) for twelve building materials. The results indicate a linear relationship between the H-SSA and moisture content, as expressed in Equation (1). The *x*-axis represents the moisture contents corresponding to monolayer coverage within each material, illustrating intervals for monolayer sorption. The gravimetric H-SSAs of the investigated building materials range between 5,900 and 459,000 m^2 kg^{-1}, with the highest values observed for bio-based materials (95,500 – 459,000 m^2 kg^{-1}), which generally exhibit high sorption dynamics. Conversely, mineral building materials show lower H-SSA (5,900 – 53,000 m^2 kg^{-1}), with the exception of mineral CS (65,000 – 156,000 m^2 kg^{-1}). The bio-composite hempcrete materials exhibit average H-SSA (61,000 – 205,000 m^2 kg^{-1}), indicating a combined effect from the mineral lime binder and bio-based hemp shives. These findings are represented in Figure 3, which utilizes a color scheme to distinguish the different material types.

Figure 3 shows that the investigated building materials display varying intervals of monolayer sorption, resulting in a range of estimated H-SSA values. To further elucidate these findings, Table 2 presents the monolayer moisture contents for each material by adsorption and desorption at 20% RH and 47% RH,

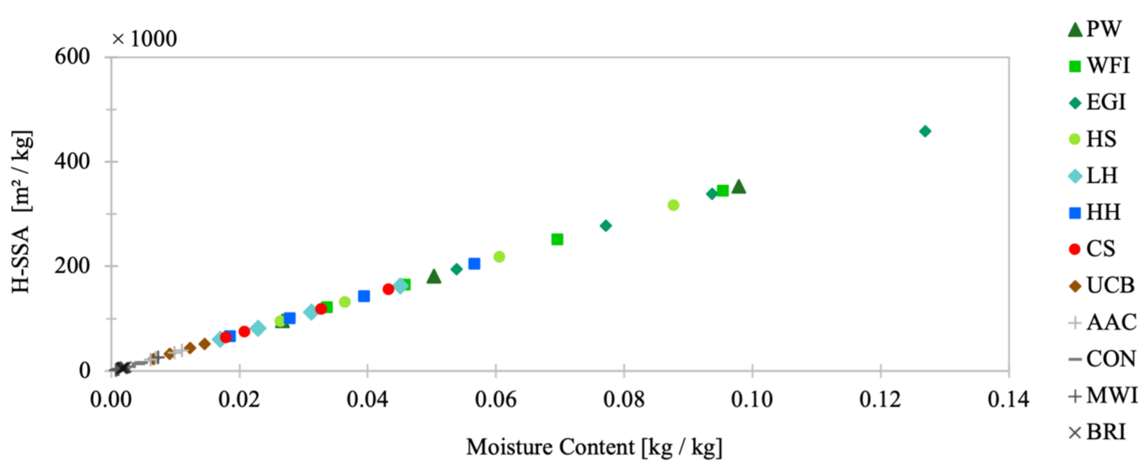

Figure 3. Hydratable specific surface area (H-SSA) in gravimetric units [m² kg^{-1}] as a function of moisture content (shown for each material at four vapor sorption points – Ads-20, Ads-47, Des-20, and Des-47; see Figure 2 for definition of points).

respectively. The bio-based materials (PW, WFI, EGI, and HS) exhibit the largest range of monolayer moisture contents, indicative of their high sorption dynamics. In this study, the upper RH boundary for potential monolayer capacity is set to 47% RH. However, if there is no dominant content of swelling clay in the given materials, the monolayer interval could be reduced from 47% RH to 34% RH [6].

Table 2. Moisture contents (Ads/Des; 20/47% RH) for the twelve building materials and their respective ranges, marking the estimated monolayer sorption.

Material	Monolayer moisture content [kg kg^{-1}]				
	Ads, 20% RH	Des, 20% RH	Ads, 47% RH	Des, 47% RH	Range ΔMC
PW	0.027	0.050	0.050	0.098	0.071
WFI	0.034	0.046	0.070	0.095	0.062
EGI	0.054	0.077	0.094	0.127	0.073
HS	0.026	0.037	0.061	0.088	0.061
LH	0.017	0.023	0.031	0.045	0.028
HH	0.019	0.028	0.040	0.057	0.038
CS	0.018	0.021	0.033	0.043	0.025
UCB	0.007	0.009	0.012	0.015	0.008
AAC	0.006	0.007	0.010	0.011	0.005
CON	0.002	0.003	0.004	0.005	0.003
MWI	0.001	0.007	0.001	0.001	0.007
BRI	0.002	0.002	0.002	0.002	0.001

3.2. Volumetric Hydratable Specific Surface Area (H-SSA)

A more intuitive understanding of the magnitude of hydratable surfaces in building elements can be expressed volumetrically, as building elements are commonly assessed by volume. To this end, two versions of the volumetric H-SSA have been presented. Figure 4 displays the moisture content on the x-axis expressed volumetrically in kg m^{-3}, while Figure 5 illustrates the H-SSA on the y-axis expressed volumetrically in km^2 m^{-3}. It should be noted that a figure with both volumetric axes has not been included,

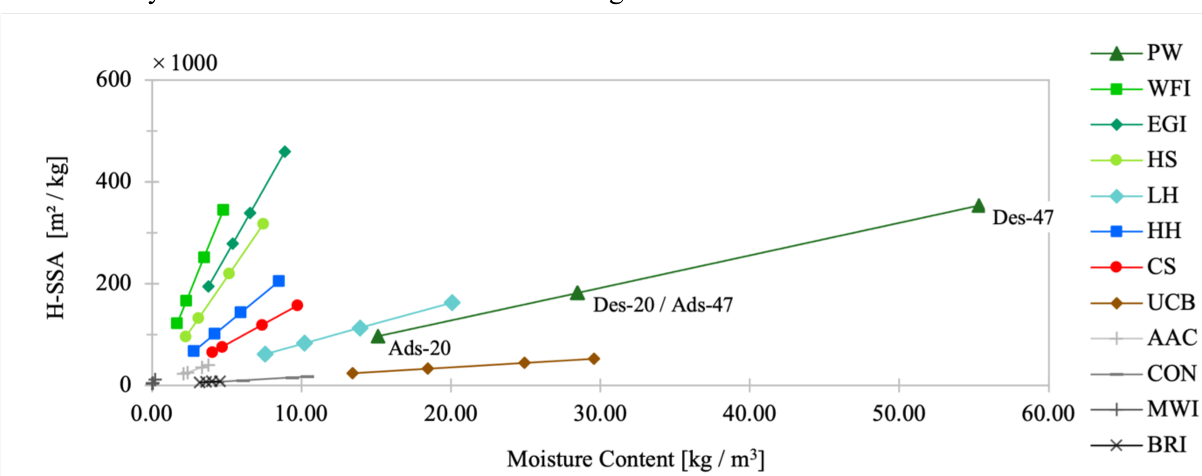

Figure 4. Hydratable specific surface area (H-SSA) in gravimetric units [m² kg^{-1}] as a function of volumetric moisture content [kg m^{-3}].

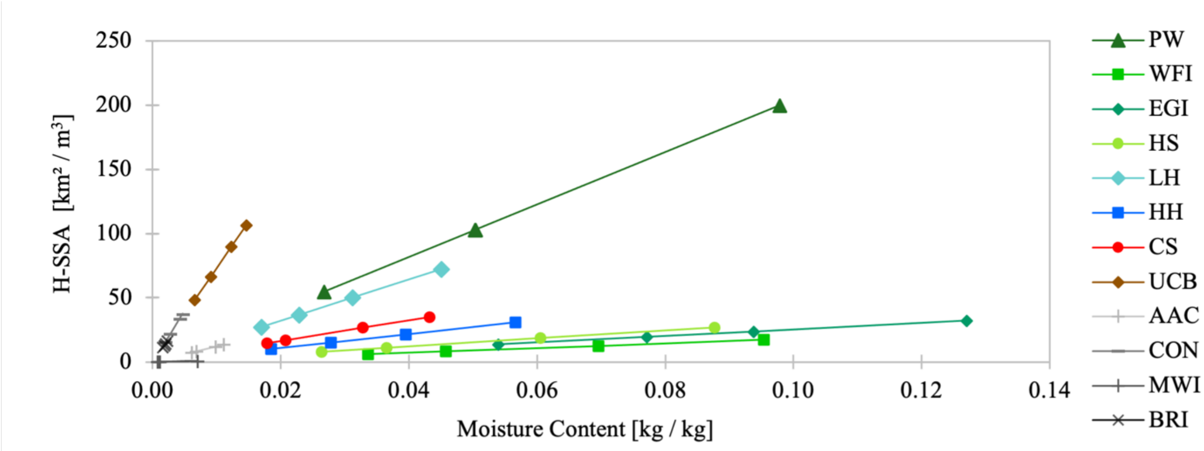

Figure 5. Hydratable specific surface area (H-SSA) on a material volume basis [km² m^{-3}] as a function of gravimetric moisture content [kg kg^{-1}].

as it displays the same linear relationship observed in Figure 3 and would make it difficult to discern variations between the different materials.

In Figure 4, the volumetric moisture content exhibits a dependence on two factors: bulk density and hygroscopicity. The highest moisture contents are observed in high-density materials such as PW and UCB, which are also highly hygroscopic. In contrast, mineral materials such as CON and BRI have higher densities but lower moisture contents due to their more hydrophobic nature. Bio-based materials such as WFI, EGI, and HS are highly hygroscopic, yet exhibit more limited monolayer moisture content due to their low densities. The hempcretes demonstrate the impact of material composition, as a larger contribution of hemp shives decreases density and subsequently reduces the volumetric moisture content, despite presenting higher gravimetric moisture content.

Figure 5 portrays the magnitude of H-SSA within a cubic meter of building materials, spanning several square kilometers (0.1 – 200 km^2 m^{-3}). In comparison, Aalborg has an area of 50.7 km^2. The conclusions drawn from Figure 4 are further reinforced by Figure 5, as both density and hygroscopicity play influential roles in the estimation of H-SSA. The highest volumetric H-SSA is observed for PW, followed by UCB and LH, owing to their high densities and hygroscopicities. Interestingly, despite exhibiting high sorption dynamics, fibrous and bio-based materials such as WFI, EGI, and HS demonstrate similar H-SSA as mineral-based materials such as BRI, CON, and AAC; these range from 6,000 to 37,000 km^2 m^{-3}.

3.3. Relating the Hydratable Specific Surface Area (H-SSA) to bulk density

Bulk density and the hydratable specific surface area (H-SSA) of materials are interrelated properties. Higher bulk density indicates that more material is packed within a given volume, which results in a lower H-SSA. Conversely, a lower bulk density indicates that there is less material packed within a given volume, leading to a higher H-SSA. While it is generally true that a higher bulk density will lead to a lower H-SSA, this correlation is not always straightforward, as illustrated in Figure 5, as the packing of the material can greatly influence the H-SSA. For example, materials with irregularly shaped particles or high levels of porosity can have a high bulk density but still exhibit a high H-SSA due to the complex packing arrangement of their particles. Similarly, materials with regular particle shapes and low porosity may have a lower bulk density but still present a lower H-SSA due to the tightly packed structure of the particles. Thus, the relationship between bulk density and H-SSA is not absolute, and other factors such as particle size and shape, porosity, and surface chemistry must also be considered when assessing the sorption dynamics of building materials.

In this study, the relationship between bulk density and hydratable specific surface area (H-SSA) has been investigated for the twelve investigated building materials. The bulk density and gravimetric H-SSA values (determined through desorption at 20% relative humidity) have been plotted in Figure 6 to explore the potential dependency between them. Interestingly, the results indicate that there is no immediate correlation between bulk density and H-SSA, either across all twelve building materials or for individual material types such as bio-based and mineral materials. However, a connection can be observed solely in the gravimetric H-SSA values, as indicated by Figure 3. Specifically, the bio-based materials including bio-composite exhibit H-SSA values exceeding ~80,000 m^2 kg^{-1}, while the mineral building materials display H-SSA values below ~80,000 m^2 kg^{-1}; this been illustrated by the dashed line in the figure. Within the mineral materials, only CS exhibited H-SSA values closer to the bio-based materials, while the remaining mineral materials presented significantly lower H-SSA values.

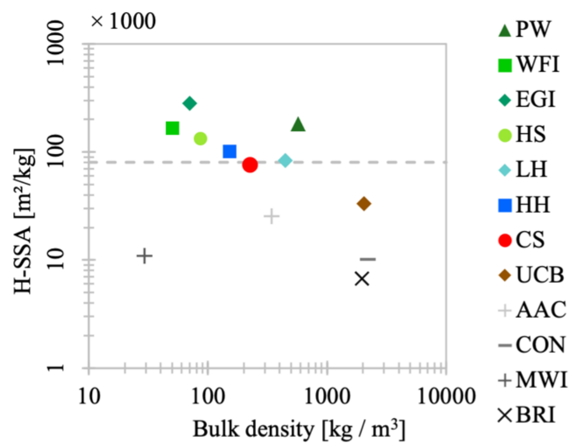

Figure 6. Hydratable specific surface area (H-SSA) as a function of bulk density at dry state. The gravimetric H-SSA has been identified by desorption at 20% RH.

4. Conclusion

The likely range of hydratable specific surface area (H-SSA) for building materials can be estimated from water vapour sorption isotherms. Obtained H-SSA for 12 different building materials ranged from 5,900 to 459,000 m^2 kg^{-1}, with the smallest values obtained for conventional mineral-based materials like brick, mineral wool insulation and concrete.

The highest H-SSA values correspond to the typical area of a building plot (e.g. 500 m^2) per one gram of dry material, and the typical area of an agricultural field in Denmark (e.g. 500,000 m^2 = 50 hectare) per kg of dry material. This well illustrates and help explains the enormous moisture regulating potential of many natural and/or bio-based building materials.

We recommend, if possible, to give H-SSA as a range representing water vapour ad-and desorption at between 20 and 47% RH, namely the monolayer interval. If giving H-SSA for only one condition, the condition of H-SSA should be precisely specified, e.g. H-SSA (Des-20; estimated from the primary desorption isotherm at 20% relative humidity).

In perspective, the presented concept of H-SSA seems promising to help explain and classify building materials in regard to their physical, chemical, and biological surface/pore-network controlled functions, including moisture regulating potential, the retainment and release of volatile toxic chemicals, and the risk for e.g. mould growth. As sorption dynamics are influenced by multiple parameters, such as particle size, shape and porosity, H-SSA derives a more representative measure of physical structure than bulk density alone.

In this study, the upper RH boundary for potential monolayer capacity is set to 47% RH. However, if there is no dominant content of swelling clay in the given materials, the monolayer interval should be reduced from 47% RH to 34% RH.

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