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An inverse modelling approach to estimate the hygric parameters of clay-based masonry during a Moisture Buffer Value test

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ABSTRACT

This paper presents an inverse modelling approach for parameter estimation of a model dedicated to the description of moisture mass transfer in porous hygroscopic building materials. The hygric behaviour of unfired clay-based masonry samples is specifically studied here and the Moisture Buffer Value (MBV) protocol is proposed as a data source from which it is possible to estimate several parameters at once. Those include materials properties and experimental parameters. For this purpose, the mass of two clay samples with different compositions is continuously monitored during several consecutive humidity cycles in isothermal conditions. Independently of these dynamic experimental tests, their moisture storage and transport parameters are measured with standard steady-state methods.

A simple moisture transfer model developed in COMSOL Multiphysics is used to predict the moisture uptake/release behaviour during the MBV tests. The set of model parameters values that minimizes the difference between simulated and experimental results is then automatically estimated using an inverse modelling algorithm based on Bayesian techniques. For materials properties, the optimized parameters values are compared to values that were experimentally measured in steady state. And because a precise understanding of parameters is needed to assess the confidence in the inverse modelling results, a sensitivity analysis of the model is also provided.

1. Introduction

Clay has been used as a construction material since man has started building. In 2012 UNESCO released an inventory of Earth construction heritage sites [1]. It shows the immense legacy of earth construction and earth architecture around the world. These sites demonstrate how durable this material can be. In modern times earth has to compete with materials such as concrete and due to its natural variability, earth is often considered as a primitive material not fit for modern construction. However, earth based masonry and renders have many qualities that are becoming more and more important in the context of global climate change and the challenge to reduce carbon emissions. The choice of using earth as a construction material varies depending on the economical situation of a country. In developing countries earth is a cheap material that can often be sourced close to the building site making it the first choice for economical reasons. In richer industrialized countries, earth is chosen for its sustainable, highly hygroscopic and aesthetic qualities [2].

Clay-based materials show high moisture storage capacity through surface adsorption and capillary condensation effects in the hygroscopic domain. Such phenomena coupled with moisture transport inside the porous structure are stated to offer a regulation capacity of the indoor air humidity [3], improving comfort for occupants [4–6]. One way to quantify this regulation behaviour is to evaluate the moisture buffer capacity, i.e. the moisture exchange capacity under a dynamic exposure to ambient relative humidity (RH) cycle. The relative humidity variations can be caused either by temperature change of the ambient air or through changing the amount of moisture in it.

The NORDTEST project [7] has been one of the first attempts to find a consensus for an experimental protocol able to adequately characterize the buffer capacity through the definition of a global

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parameter called the Moisture Buffer Value (MBV). Beside the direct humidity regulation that is evaluated by the MBV at material scale, the buffer performance of hygroscopic materials also causes latent heat effects whose impact on energy balance is only partially assessed [8].

Along with the will to characterize porous hygroscopic and capillary materials experimentally, the modelling of their behaviour has progressed substantially in the last decades [9–12]. Indeed, Heat Air and Moisture (HAM) models which deal with detailed hygrothermal analysis of porous materials have improved in accuracy through the development of computer power and a better knowledge of the involved phenomena. Many HAM computer models and associated software have been developed for building applications and some have been commercialized [13,14]. The main difference between the models is in the description of the moisture flows that can have several levels of complexity, ranging from diffusivity models using moisture content as driving potential to conductivity models using the actual thermodynamic driving potential and separated liquid and vapour flows [15]. All these models rely on material and boundary condition parameters, most of them being time consuming to obtain.

The computation of temperature and moisture content fields in building materials, from the known parameters and boundary conditions forms a *direct HAM problem* [16]. This approach is the most common in Building Physics, where the aim is often to predict the behaviour of material assemblies under various climatic solicitations. The validity of such approaches relies on the quality of characterization for the hygrothermal properties of the material. In contrast to direct modelling process, there exist several methods that allow parameter estimation from temperature and moisture content field measurements, which establishes a new kind of *inverse HAM problem*. Among inverse modelling methods, the Bayesian approaches are becoming more and more popular in environmental models. In Bayesian optimization, parameters are not unknowns with a single value to determine, but stochastic variables whose distributions have to be specified. The distribution given before estimation is called '*a priori*' and the distribution given after integration of the experimental data is called 'a posteriori'. Historically, the emergence of the Markov Chain Monte Carlo (MCMC) simulations with the Random Walk Metropolis algorithm as first widely used approach [17] have greatly simplified the estimation of posterior distribution of parameters. Recently, Ter Braak [18] developed the Differential Evolution-Markov Chain (DE-MC) method, able to run several Markov chains in parallel with a so called 'genetic' algorithm for the sampling process, improving the parameter space exploration efficiency. The Differential Evolution Adaptive Metropolis (DREAM) algorithm [19,20] is an evolution of the DE-MC, able to automatically tune the scale and orientation of the proposed parameter distributions (i.e. self-adaptive randomized subspace sampling) during the evolution towards posterior distribution. A good review about Bayesian approaches and inverse modelling algorithms evolution can be found in Ref. [21].

The goal of this paper is to illustrate the use of a MCMC sampler to estimate the parameters of a HAM model in an inverse modelling problem. For this purpose, we propose to study the applicability of the MBV protocol as the source of experimental data to estimate hygric properties of porous construction materials. Specifically, the mass variation of different clay-based samples is measured experimentally during a MBV test. In parallel, their moisture storage and transport properties are measured in steady-state conditions. The DREAM algorithm is then coupled to a simplified moisture transfer model which simulates the moisture exchange of samples. The parameters sampling process consists in automatically tuning the HAM model in order to match experimental mass variation by testing various combinations of parameters values and evaluating the resulting model efficiency. Eventually, the inverse modelling approach can propose a 'best parameters set' which minimizes the difference between the simulated and the measured moisture uptake/release of sample. Four parameters are estimated in this paper; two are directly related to the material and two others linked to experimental conditions. For the first category, the best estimated parameters resulting from the inverse modelling approach can be compared to their corresponding value measured in steady-state.

The questions arising from this study are: (1) how the different model parameters interact during the MBV cycle, with possible correlations; (2) is it reliable to use this single dynamic experiment to retrieve several parameters at once with the inverse modelling method; (3) do the dynamic conditions of the MBV test offer a more 'realistic' configuration for material properties assessment?

2. The Moisture Buffer Value

The need for a standardized parameter to characterize the moisture buffering capacity of materials led to the definition of the Moisture Buffer Value (MBV) during the NORDTEST project [4] together with the proposal of a dynamic experimental protocol for materials classification. The practical MBV is defined as: "the amount of water that is transported in or out of a material per open surface area, during a certain period of time, when it is subjected to variations in relative humidity of the surrounding air" [7]. Concretely, the samples are subjected to cyclic step changes in relative humidity (RH) at a constant temperature of 23 °C and are weighted regularly. The cycle is composed by moisture uptake during 8 h at high RH followed by moisture release 16 h at low RH and is repeated until constant mass variation between 2 consecutive cycles is reached. The practical MBV in kg/(m^2 %RH) is then given by Eq. (1).

$$MBV_{practical} = \frac{\Delta m}{A \cdot \Delta RH} \tag{1}$$

where Δm is the mass variation during the 8 h absorption phase or the 16 h desorption phase in one complete cycle, A (m^2) is the total exchange surface and ΔRH is the difference between the high and low relative humidity of the cycle. This experimental value is a direct measurement of the amount of moisture transported to and from the material for the given exposure cycle. In the original protocol, the cycle is fixed to a 75/33%RH scheme.

A theoretical value of the MBV, called MBV_{ideal}, can be computed analytically using semi-infinite solid theory and Fourier series without transfer resistance at exchange surface. There is always a disagreement between measured and analytically calculated due to the dynamic nature of the experimental protocol, the film resistance on specimen exchange surface and deviations from the typical step transitions. However is has been shown in McGregor et al. [22] that a good agreement can be found between measured and calculated MBV when reducing the film resistance in the dynamic test and improving the precision of the steady state measured properties.

3. Materials and methods

3.1. Samples

Two different soils were used for the experimental measurement. The *Gr* soil is a natural soil extracted from the Wealden clay group in the UK. The natural soil had high clay content, so 50% by weight of fine builders sand was added. The final particle size distribution consisted of 18% of clay, 24% of silt and 58% of sand. The