Investigation of Water Vapour Transport Properties of Gypsum Using Genetic Algorithm

Z. Pavlík, J. Žumár, M. Pavlíková, J. Kočí, and R. Černý

***Abstract*—**Water vapour transport properties of gypsum block are studied in dependence on relative humidity using inverse analysis based on genetic algorithm. The computational inverse analysis is performed for the relative humidity profiles measured along the longitudinal axis of a rod sample. Within the performed transient experiment, the studied sample is exposed to two environments with different relative humidity, whereas the temperature is kept constant. For the basic gypsum characterisation and for the assessment of input material parameters necessary for computational application of genetic algorithm, the basic material properties of gypsum are measured as well as its thermal and water vapour storage parameters. On the basis of application of genetic algorithm, the relative humidity dependent water vapour diffusion coefficient and water vapour diffusion resistance factor are calculated.

***Keywords*—**Water vapour transport, gypsum block, transient experiment, genetic algorithm.

I. Introduction

Properties characterising the water vapour transport and storage in porous building materials represent necessary information for optimal design and construction of buildings. Knowledge of these material parameters is significant especially for materials of building envelope, nominally for thermal insulations, walling blocks, air tight layers, plasters, etc.

In the hygroscopic range, where the transport of water vapour is dominant mode of moisture transfer, the moisture storage parameters are called sorption and/or desorption isotherms [1]-[3]. They express the dependence of the moisture content in a material on the ambient relative humidity.

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One must take into account also fact that adsorption of water vapour is an exothermic process hence the amount of vapour adsorbed at equilibrium must decrease with increasing temperature [4], [5]. In materials research are these storage parameters measured in almost the same form for many decades using dessicator method that is sometimes called climate box method [6]. Since this method can take a relatively long time, new sophisticated methods were developed for sorption isotherms measurement. Here, especially gravimetric sorption microbalance method also called dynamic vapor sorption method is the most often applied technique [6]. This method allows determination of adsorption as well as desorption isotherms within short time (typically one or two days depending on materials of inner structure) and in dependence on temperature.

Compared to water vapour storage functions measurement that is presently well established in materials research, assessment of material parameters characterising the water vapour transport remains still an open question. For the measurement of water vapour transport properties, the steady state cup method in different experimental arrangements is the most often used technique. This method is the most popular for its simplicity and is generally considered as reliable and relatively accurate [7].

As the intensive research on water transmission proved, the water vapour diffusion properties depend on relative humidity in material. Therefore, the existing standards based on cup method require measurement in several pairs of relative humidity [8], [9]. However, from these measurements only step-wise relationship between diffusion parameters and relative humidity is accessed within highly time-consuming experiments.

On this account we referred in [10], [11] about new combined computational-experimental approach for the determination of water vapour diffusion properties of porous building materials in dependence on relative humidity. This methodology is based on measurement of relative humidity profiles and their inverse analysis using computational modelling involving genetic algorithms. Since the first achieved results are very promising, we present in this paper further application of this method for the assessment of water vapour transport properties of gypsum block.

II. Experimental

A. Studied Material

The studied gypsum block is product of Czech company GYPSTREND Ltd. The block is based on grey gypsum that is modified by plasticizer, hydrophobic admixture, and expanded perlite. Plasticizer Polyfor is product of Forchem Ltd., Czech Republic. It is liquid substance that is originally used for lime-cement mortars as plasticizer and air-entraining agent having stabilisation effect. Hydrophobic admixture MH 1107 was manufactured by Dow Corning-Construction Chemical. It is unique product on the basis of polymethylhydrogen siloxane designed for hydrophobic treatment of gypsum plaster boards. Expanded perlite EP 150 is product of Pertlit, Ltd., Czech Republic. It has bulk density 150 kg/m^3, granularity 0 – 1 mm and thermal conductivity 0.042 W/m K. Composition of researched gypsum block is given in Table I.

TABLE I
COMPOSITION OF TESTED GYPSUM BLOCK

Water/gypsum ratio	Mass % of gypsum		
	Polyfor	MH 1107	Perlite EP 150
0.96	1.0	0.5	10.0

B. Material Properties of Gypsum Block

Computational application of genetic algorithm requires data on material parameters of investigated material. On that account, measurement of matrix density, bulk density, total open porosity, pore size distribution, thermal properties, sorption and desorption isotherms were done.

Matrix density was measured by helium pycnometry using apparatus Pycnomatic ATC (Thermo). Bulk density was accessed using gravimetric method by weighing the sample mass and measurement its linear dimensions. From the known values of matrix density and bulk density, the total open porosity was measured. The basic material properties are summarised in Table II. The accessed porosity is very high what brings to the studied gypsum block good thermal insulation properties.

TABLE II
BASIC MATERIAL PROPERTIES OF TESTED GYPSUM

Bulk density (kg/m^3)	Matrix density (kg/m^3)	Total open porosity (-)
516	2183	0.76

The porosity measurements were performed on dried samples using apparatuses Pascal 140 and 440 (Thermo) working on mercury intrusion principle [12]. The physical basis of this measurement results from the assumption that the non-reactive and non-wetting liquid (in our case mercury) will not penetrate pores until sufficient pressure is applied to force its entrance. As narrow pores must be filled up, such high pressure must be applied [13]. The results of pore size distribution measurement are given in Figs. 1, 2. We can see very uniform behaviour of gypsum having the highest pore volume in the range of 1.0 – 7.0 μm.

Among the thermal properties, thermal conductivity, specific heat capacity and thermal diffusivity were measured for the dried material samples. For that purpose we used commercial device ISOMET 2104 (Applied Precision, Ltd.). ISOMET 2104 is a multifunctional instrument for measuring thermo-physical parameters which is based on the application of an impulse technique and is equipped with various types of optional probes [14]. In our measurement we used contact surface probe, whereas the samples size was 70/70/100 mm. Thermal parameters are given in Table III.

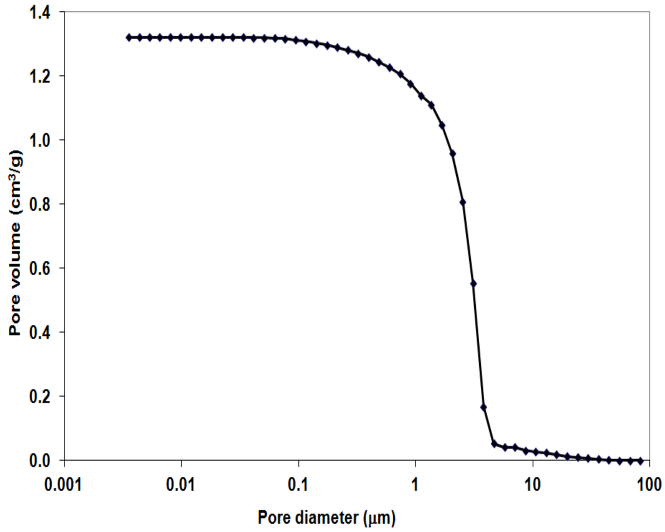

Fig. 1 Pore size distribution – cumulative curve

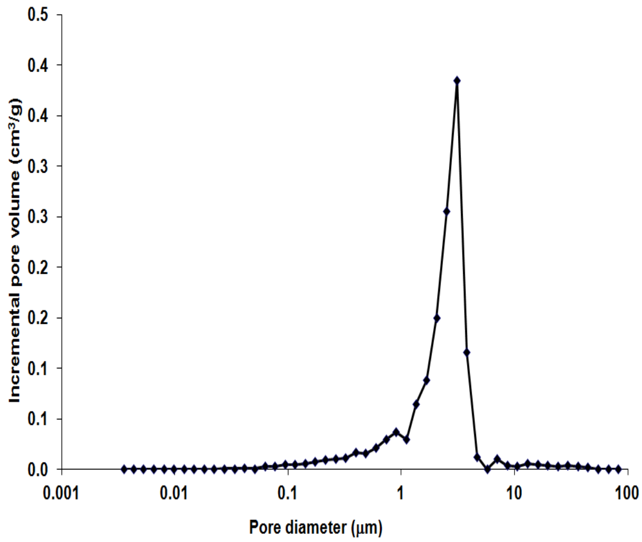

Fig. 2 Pore size distribution – distribution curve

TABLE III
THERMAL PARAMETERS OF TESTED GYPSUM

Thermal conductivity (W/m K)	Specific heat capacity (J/kg K)	Thermal diffusivity (m^2/s)
0.21	2 740	1.49E-07

Sorption and desorption isotherms were measured at temperature 25°C using dynamic sorption device DVS-Advantage II (Surface Measurement Systems Ltd.). The instrument measures the uptake and loss of vapour gravimetrically, using highly precise balances having resolution of 0.1 μg. The partial vapour pressure around the sample is generated by mixing the saturated and dry carrier gas streams using electronic mass flow controllers [15]. The humidity range of the instrument is 0 – 98% with accuracy ± 0.5% at temperatures 5 – 60°C. In this way, the temperature dependence of vapor adsorption/desorption can be measured as well. In Fig. 3 the history of the measuring process is presented. Sorption and desorption isotherms are given in Fig. 4. The sorption capacity is typically very low. However, material exhibits hysteretic behaviour.

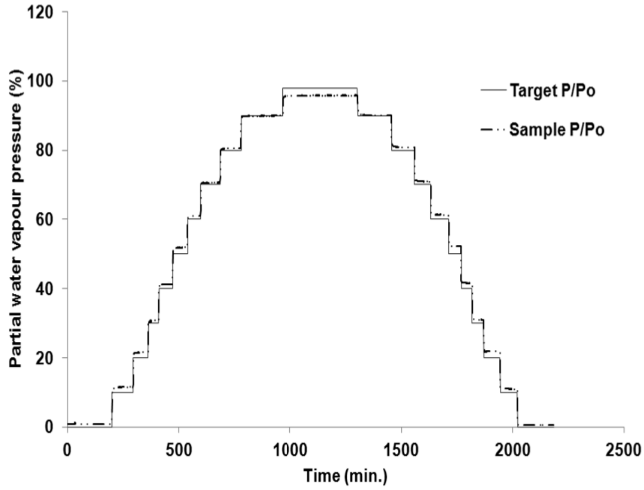

Fig. 3 History of dynamic sorption experiment

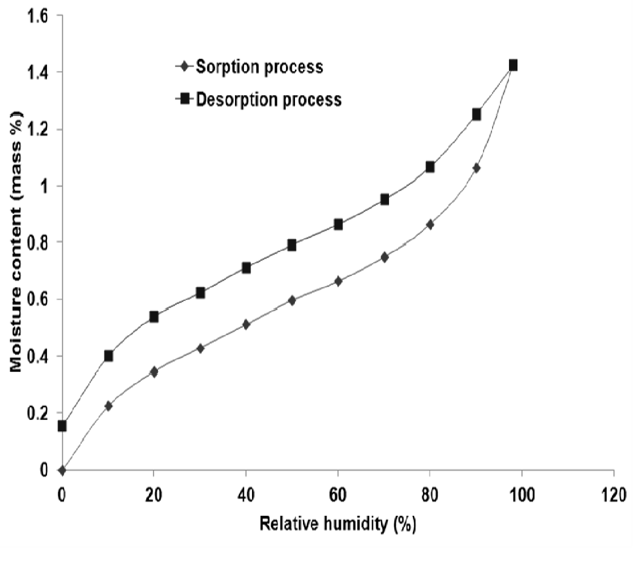

Fig. 4 Sorption and desorption isotherm of gypsum

C. Transient Experiment

For application of computational inverse analysis, knowledge on relative humidity distribution along the sample length which is oriented in parallel to water vapour transport must be known. For that purpose, experimental apparatus that was devised originally at our laboratory and firstly introduced in [11] was used. It consists of two airtight chambers that are separated by measured rod shape sample having length 280 mm and cross section 105 x 70 mm. The sample was on all lateral sides provided by epoxy resin in order to ensure 1-D water vapour transport only through its open sides. In the first chamber, saturated water solution of K_2SO_4 was placed for simulation of high relative humidity typically about 98%. In the second chamber, silica gel that maintained constant relative humidity 4% was used. In this way, simulation of gradient of partial water vapour pressure was done. The increase of the silica gel mass due to the absorption of water vapour transported through the sample was continuously monitored by automatic balances.

For monitoring of relative humidity fields, the capacity hygrometric micro-sensors from Ahlborn, Germany, were used. They were placed into the before bored holes in specific distances along the sample length in such manner that no disturbance of water vapour flux through the sample occurred. The schematic view of the transient experiment is introduced in Fig. 5.

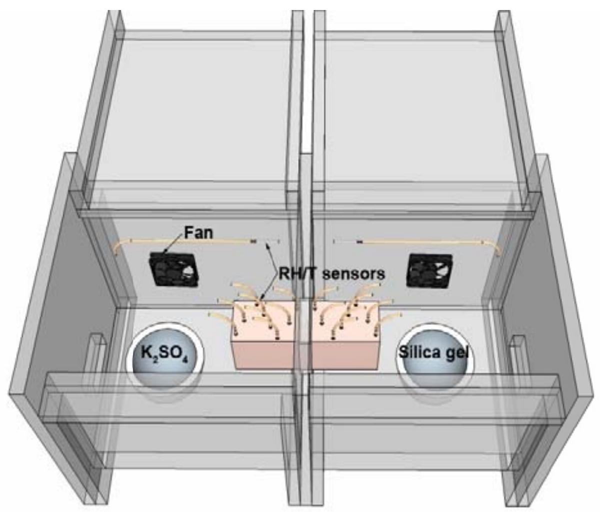

Fig. 5 Scheme of the transient experiment

III. Computational

The measured relative humidity profiles were analysed using computer code HEMOT [9] and GRADE genetic algorithm [16].

HEMOT is numerical simulation tool developed in our laboratory for simulation of coupled moisture and heat transport in building materials and structures. It allows solution of 1D and 2D problem, whereas the hygrothermal variables can be accessed as functions of space and time. The mathematical formulation of coupled heat and moisture transport equations is basically done according to Künzel [17] and the code works on the basis of finite element method.

Genetic algorithms belong to a group of evolution algorithms, which includes also evolution strategies and genetic programming. At present, genetic algorithms are one of the most modern optimization methods available. They follow an analogy of processes that occur in living nature within the evolution of live organisms during period of many millions of years. In genetic algorithm, a population of individuals (chromosomes), which encode candidate solutions to an optimization problem, evolves toward better solutions. The evolution usually starts from randomly generated population and happens in generations. In each generation, the fitness function of every individual in the population is evaluated, multiple individuals stochastically selected from the current population (based on their fitness) and modified using genetic operators (cross-over, mutation) to form a new population. The new population is then used in the next iteration of the algorithm. Commonly, the algorithm terminates when either a maximum number of generations has been produced (a satisfactory solution probably have not been reached), or a satisfactory fitness level has been reached for the population. The details on the GRADE algorithm and its algorithmic scheme are given in [10], [11].

Within the performed calculations, the optimised water vapour diffusion resistance factor as function of relative humidity was found by the use of GRADE code and verified by agreement between data calculated by HEMOT code and measured within the transient experiment. From the accessed water vapour resistance factor, the water vapour diffusion coefficient was calculated according to the equation

$$D = \frac{D_a}{\mu}, \quad (1)$$

where μ (-) is water vapour diffusion resistance factor, D (m^2/s) is water vapour diffusion coefficient, D_a (m^2/s) water vapour diffusion coefficient in air. Since parameters D, D_a exhibit similar pressure and temperature dependence, the following formula [18] was considered for calculation of water vapour diffusion coefficient in air

$$D_a = 2.3 \cdot 10^{-5} \frac{p_0}{p} \left(\frac{T}{273} \right)^{1.81}. \quad (2)$$

Here, p_0 (Pa) is barometric pressure within the transient experiment, p (Pa) barometric pressure at the sea level, T (K) Kelvin temperature.

IV. Results and Discussion

Fig. 6 demonstrates the mass increase of silica gel due to the water vapour absorption. The data exhibit linear behaviour. However, one can recognize two different slopes of mass increase. At the beginning of the experiment, the mass increase was faster which means that the water vapour flux through the sample was bigger. This can be attributed to the effect of surface diffusion. After approximately 1 h, the inner surface of gypsum pores was fully covered by water vapour molecules, and no surface diffusion took place.

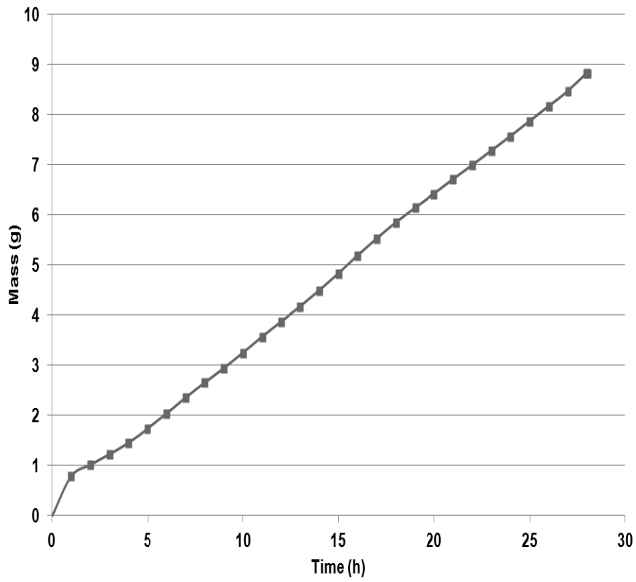

Fig. 6 Mass increase of silica gel

Typical relative humidity profiles measured within the transient experiment are presented in Fig. 7. One can see that the experiment was performed until the steady-state water vapour flux was reached.

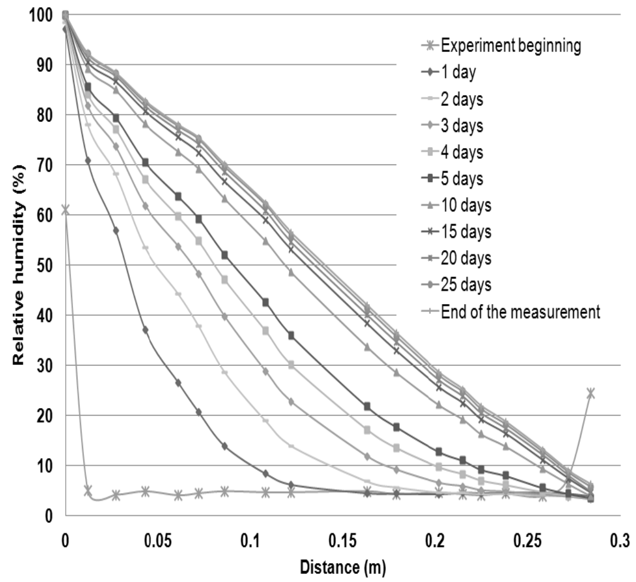

Fig. 7 Typical relative humidity profiles measured within the transient experiment

Relative humidity profiles calculated by HEMOT code using the optimised water vapour diffusion resistance factor accessed within the application of GRADE algorithm are given in Fig. 8. We can see relatively good agreement between measured and calculated data what basically validates the calculated water vapour transport properties of studied gypsum block.

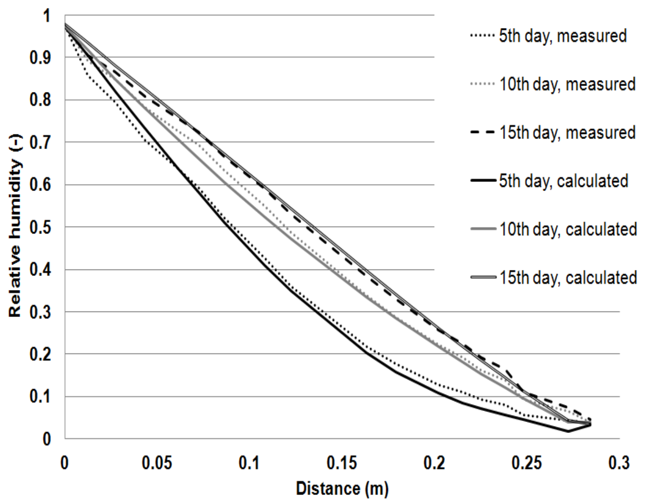

Fig. 8 Comparison of measured and calculated relative humidity profiles

Water vapour transport properties of researched gypsum are given in Figs. 9, 10. One can observe their high dependence on relative humidity what is very significant finding from the point of view of the practical use of the studied material.

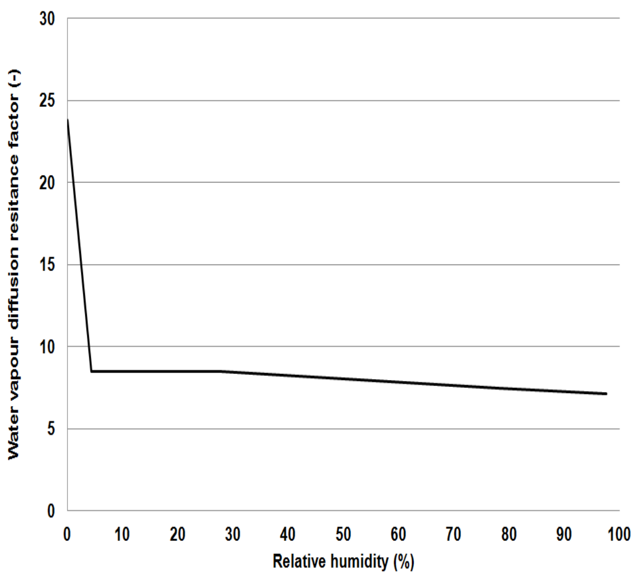

Fig. 9 Water vapour diffusion resistance factor of gypsum block

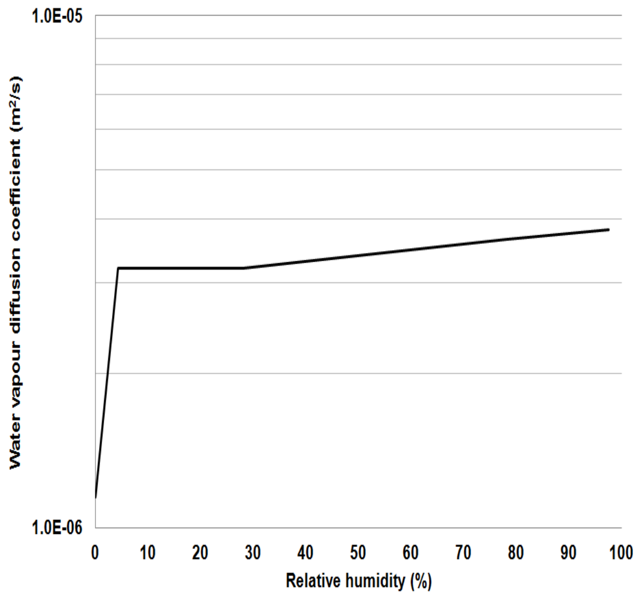

Fig. 10 Water vapour diffusion coefficient of gypsum block

V. Conclusion

In this paper, a combined experimental/computational technique was used for the assessment of water vapour transport properties of gypsum block. The water vapour parameters were determined as functions of relative humidity, what represents valuable information for the application of the researched gypsum block in building practice. The measured adsorption and desorption isotherms revealed very low sorption capacity of studied material, what is beneficial for its use. The presented transient experiment and its computational evaluation can be considered as a further step to wider utilization of the developed technique in materials research.

Acknowledgment

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