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Anderberg, Anders; Wadsö, Lars

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2

LUND UNIVERSITY

PO Box 117
221 00 Lund
+46 46-222 00 00

LUND INSTITUTE OF TECHNOLOGY
LUND UNIVERSITY

Division of Building Materials

A computer-based programme that simulates the drying of self-levelling flooring compounds

Anders Anderberg and Lars Wadsö

TVBM-7191 Lund 2007

Lund Institute of Technology
Division of Building Materials
PO Box 118

SE-221 00 LUND

Tel: 046-2227415
Fax: 046-2224427
www.byggnadsmaterial.lth.se

Preface

A computer based programme, Maxdry, predicting drying of self-levelling flooring compounds has been developed at Building Materials, Lund University in close cooperation with Maxit Group AB. The present report describes the programme: its structure, limitations and assumptions. The laboratory work determining input data to the programme was conducted during 2003-2006 and the programme was written during 2005-2006. The programme is written in Matlab R2006b. If the end-user does not have Matlab, a compiled version (using Matlab Compiler 4.5) of the programme can be used together with an external function library.

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Abbreviations and symbols

SLC	Self-levelling flooring compound.
RH	Relative humidity (-) or (%), ratio of actual vapour content (g m^{-3}) and vapour content at saturation (g m^{-3}) at the present temperature.
MC	Moisture content (moisture ratio) as % by dry mass (10% RH at 20 °C), which generally corresponds to oven drying at 40 °C.
CM	Calcium carbide method, a method where the moisture content is measured in materials as % of wet mass.
MTC	Mass transfer coefficient (g m^{-2}s^{-1}Pa^{-1}).
w/b	Water binder ratio, ratio between mass of water and mass of binder.
v	Water vapour content in air (g m^{-3}).
Δv	Difference in water vapour content (g m^{-3}).
D_v	Diffusion coefficient with water vapour content as potential (m^{2}s^{-1}).
R	Universal gas constant (8.314 JK^{-1}mol^{-1}).
E_a	Activation energy (JK^{-1}mol^{-1}).
α	Degree of hydration, ratio of heat produced at time t and heat produced when all binder is reacted, as measured with isothermal calorimetry.
Q	Heat (Jg^{-1} material), proportional to extent of reaction.
P	Thermal power (Wg^{-1} material), proportional to the rate of reaction.

Contents

Chapter 1

Introduction

Moisture in materials is an important issue both regarding the status of a construction part or a whole building. Moisture influences physical properties of materials such as shrinkage/swelling and strength, biological processes like mould growth as well as chemical processes like degradation of polymers in floor adhesives, and hydration reactions of inorganic binders.

Self-levelling flooring compounds are generally cast with a large excess of water due to their desired flowing properties. This excess water has to be dried out before applying a surface covering such as PVC-floorings, wooden parquets, etc., to avoid future moisture-related problems. The drying time mainly depends on the product, its layer thickness and the ambient climate (temperature, relative humidity in air, and air speed at surface).

In order to plan for the construction process it is necessary to be able to predict drying times for the materials used. This calculation programme enables the planning by predicting drying times for self-levelling flooring compounds. It may also be used as a tool to study which factors that influences the drying process and what will happen with the predicted drying time when deviations from the original plan occurs. Deviations may be changes in climate conditions, thicker or thinner layers, delayed casting date, etc.

This manual describes the calculation programme, how it is built up, and its limitations and assumptions.

Chapter 2

General description of the drying of SLCs

Drying of SLCs occurs as a result of four processes: first, evaporation from the surface to the ambient air. Secondly, self-desiccation by chemical binding of water in the hydration products. Thirdly, self-desiccation by physical binding of water in the developing pores of the material. And finally, moisture flow into the substrate and other materials in contact with the SLC.

Surface evaporation starts immediately upon mixing. Sometimes bleeding occurs, forming a water film on the surface. During this initial stage, the rate of surface evaporation mainly depends on the temperature, relative humidity (RH) and the air speed in the surrounding air. The main reaction starts within a couple of hours and the material turns from a particle suspension into a solid. During this period, the surface will gradually dry and a moisture gradient will develop through the material. The rate of surface evaporation will now depend on the moisture transport from within the material to the surface as well as temperature and RH in air, while the influence of the air speed of the surroundings only plays a minor part. As hydration proceeds, the structure of the material changes and so will the moisture transport properties.

Chemical binding of water occurs when water reacts with the binder, e.g., cement and calcium sulphate in the case of SLCs, and becomes chemically bound in the reaction products. The rate of chemical binding of water is proportional to the rate of reaction, which is a function of the temperature, the extent of reaction and the moisture state. Generally, for cementitious materials, hydration takes place as a number of complex simultaneous and competitive reactions [1].

In addition to its chemical binding, water is also physically bound to the surfaces and water menisci in the pore system. These pores generally have radii in the nanometre range. Thus they are also capable of holding capillary water at a low relative humidity according to the Kelvin equation [2], which describes the relationship between the radius of a water meniscus and the corresponding water vapour pressure. When SLCs hydrate, fine pores are developed and the material's capacity to hold hygroscopic water increases.

The fourth drying process mentioned above, moisture flow into the substrate, is usually not much discussed, but can be of importance in some applications. One example is the application of an SLC to a dry concrete substrate by renovation, where the concrete can absorb an appreciable amount of water from the SLC.

Chapter 3

Programme description

3.1 General

The present one dimensional programme cannot deal with problems in two or three dimensions. In most cases one dimension is sufficient for describing the construction, but two or three dimensional modelling is necessary when for example tiles are applied, by floor heating (non-isothermal modelling) and by odd shapes in the substrate.

In the previous chapter a short description of the drying of SLCs is given. Below follows a description of how the drying of SLCs and the factors influencing the drying are described in the simulation programme, including a description of the assumptions and limitations.

3.2 External climate conditions and surface mass transfer coefficients

The external climate conditions are given as input data to the programme by the user. Three different climate data are given, temperature, RH and air exchange rate (the programme will translate the air exchange rate into a surface resistance at the material surface).

The temperature can be entered as a function of time. A temperature change in the surrounding air will in reality quickly lead to a similar temperature change in the SLC. The programme will instantaneously change the temperature throughout the whole layer of material when the ambient air temperature changes.

The RH in the ambient climate can be entered as a function of time, analogous with the temperature. The RH in the ambient air together with the temperature determines the vapour content in the air. The difference between the vapour content in air and the vapour content in the material surface is the driving potential for the surface evaporation.

The air exchange rate can be entered as one of the following four alternatives: closed windows and doors, partly open windows, partly open windows and doors or fully open windows and doors. For the four different levels of air exchange rates, the surface MTC is assumed to correspond to an air layer of 16, 8, 5 and 3 mm respectively. The air exchange rate will mainly influence the surface mass transfer coefficient, MTC, which can be seen as a layer of stagnant air at the surface of the material. The surface MTC corresponds to a resistance of 40 m/s per mm of stagnant air at 20 °C (about 42 m/s at 10 °C) [3].

The heat of evaporation, that is cooling of the surface when water evaporates, is not taken into consideration, neither is the heat of hydration, which by thicker layers temporarily may increase the temperature significantly.

3.3 Initial hours before and during setting and hardening

During the initial hours after mixing, the product turns from a particle suspension into a solid material. As SLCs are mixed with a high w/b the moisture state will initially be very high throughout the entire thickness and a significant bleeding often occurs. The water that evaporates during the initial hours before the product sets and hardens is evenly reduced from the whole thickness. The relative humidity is assumed to be 100% throughout the whole material during the initial hours.

The time span of this period is set to be 12 hours at 20 °C. This time period is assumed to be temperature dependent according to the Arrhenius equation, describing the relation between the rate of chemical reactions and the temperature.

Chemical reactions, including chemical binding of water and physical binding of water will be simulated during this initial period. Moisture transport to substrate is not included in the present version, but is intended to be included in a future version.

3.4 Moisture transport in a material

After the initial hours, described above in section 3.3, the material is considered to be a solid where the moisture transport is described with equations and moisture transport coefficients. The material is divided into thin cells, see Figure 3.1, where the moisture transport between the individual cells is simulated using Fick's law of diffusion:

$$q = D_v \frac{\triangle v}{\triangle x}$$

where q (g $\mathrm{m^{-2}s^{-1}}$) is the moisture flow, D_v ($\mathrm{m^2s^{-1}}$) is the diffusion coefficient with water vapour as driving potential, $\triangle v$ (g $\mathrm{m^{-3}}$) is the difference in vapour content and $\triangle x$ (m) is the distance between two cells. The vapour content is here regarded as the driving potential for the moisture transport within the materials.

The diffusion coefficient, D_v, is treated as a function of the moisture state, but not as a function of the degree of hydration. The influence of temperature on the diffusion coefficient with vapour content as potential is generally small and will not be taken into consideration in the present version of the programme.

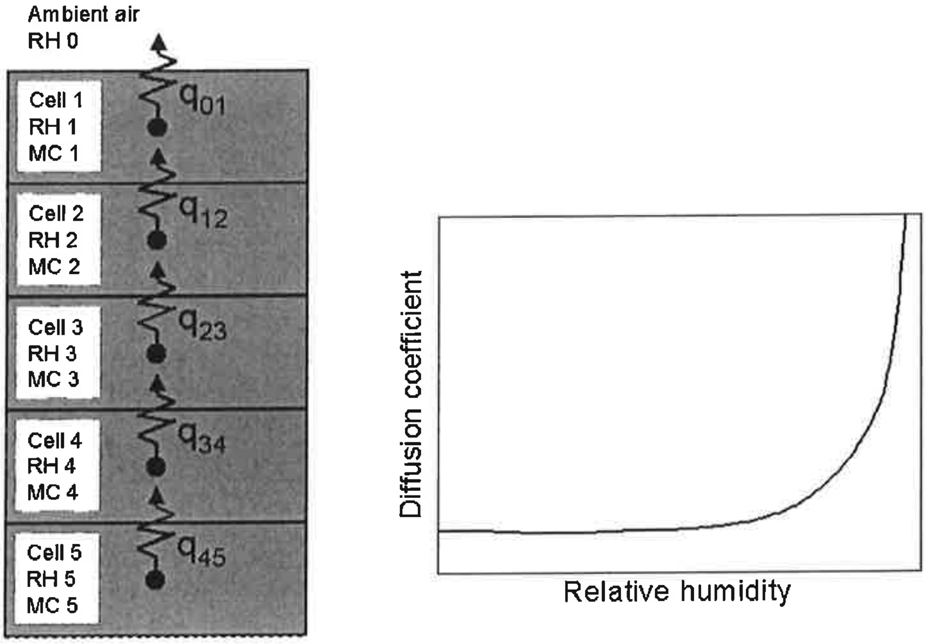

Figure 3.1: Left, schematic picture of the cell structure used in the programme for the simulation moisture transport. Right, a typical example of a diffusion coefficient where the value is strongly dependent on the relative humidity in the material. At RH above 90% the slope of the curve is generally very steep.

3.5 Surface evaporation

The rate of surface evaporation, after the initial hours is also simulated using Fick's law of diffusion. The rate of surface evaporation depends on the the surface MTC and the difference in vapour content between air and the material's surface.

3.6 Rate of reaction and chemical binding of water

The rate of reaction gives an indication of how the material structure develops in time as well as it indicates the rate of chemical binding of water. For the input data to the programme the rate of reaction has been quantified by isothermal calorimetry where the thermal power of the hydrating material is measured. The accumulated thermal power, heat, is here assumed to be proportional to the amount of chemically bound water. The rate of reaction depends on the extent of the reaction (degree of hydration), the temperature (energy of activation) and the moisture state, RH, in the material. A decrease in RH in the material means that the availability of water in the material decreases and consequently will the rate of chemical reactions decrease. The dependence of rate of reaction on RH is not fully known. For each material type it has been investigated at which RH the rate of reaction gets negligible. This RH has been set as the lowest value where chemical reactions occurs and the rate of reaction is set to increase linearly from this value up to 100% RH. This value has after a small investigation been set to 80% for the cement based SLCs and 70% RH for calcium sulphate based SLCs, although it is most probable that reactions also occur at lower RH.

The temperature dependence is described with the activation energy determined at different constant temperatures with isothermal calorimetry and evaluated with the Arrhenius equation. The activation energy is generally only suitable to use up to an α of about 0.5 for cementitious materials [4]. At higher α the reaction rate is more dependent on diffusion through hydrated layers. The present version of Maxdry will assume an E_a independent of α, although practical measurements have shown that E_a decreases when α is greater than 0.5.

Chemically bound water is the water that reacts with the binder and forms reaction products in the hydrated state. Once it is bound to the hardened structure, it is normally of no more interest. The amount of water that is chemically bound is only interesting as this contributes to the drying of the material. Chemically bound water is here defined as water left in the material when dried at 20 °C and 10% RH, which generally gives similar values as by oven drying at 40 °C.

3.7 Physical binding of moisture, moisture sorption

Physically bound water is water that is adsorbed on inner pore surfaces or condensed on water menisci formed in pores (which means that part of the pores are water filled). The physically bound water strives to stand in equilibrium with the surrounding atmosphere. Physically bound water is the water that we generally measure in our materials, either as the amount of water (moisture content determined by for example oven drying, drying over desiccants or by CM) or the state of the water (RH-method). The relation between RH and moisture content is not only different for different materials, but also depends on the degree of hydration and moisture history for a specific material.

The amount of physically bound water is described by the sorption isotherm that gives the amount of physically bound water (moisture content) as a function of RH. The sorption isotherm is slightly temperature dependent, an increase in temperature gives an increase in RH at a given moisture content. The temperature dependence is about 0,2%-units RH per °C in the RH range of 50-95% for cement based SLCs [5], that is, an increase in temperature by 1 °C results in an increase in RH by 0,2% at constant moisture content. This phenomenon is not included in the present version.

Physically bound water is here defined as water that evaporates from the material when dried at 20 °C and 10% RH. One sorption isotherm is used in the present version, determined in desorption mode after 28 days curing at 20 °C and 100%. The sorption isotherm will consequently not develop with the degree of hydration.

Moisture sorption in SLCs has a large hysteresis, that is, it shows different behaviour by drying and re-wetting. However, in the present version of the programme sorption hysteresis is not be included.

3.8 Moisture transport to other materials

Moisture transport to other materials will not be included in the present version as this version simulates drying of single layers cast on "inert" substrates. A future version of the programme is planned to include multi-layers of SLCs including the use of primers, thereby making it necessary to include moisture transport between materials. A future version may also include the possibility to add a concrete substrate, both by construction and renovation.

3.9 Surface treatment and floor covering

Surface treatments and floor coverings will not be included in the present version. A future version may include the possibility to use primers and floor coverings such as PVC-flooring, linoleum floorings, wooden parquets, etc. The influence of moisture from a floor adhesive and primers will then also be taken into consideration.

Chapter 4

Structure of the programme

The programme can be divided into several parts. An overview is given in Figure 3.1. In the user interface, the user defines input data to the programme, that is, which product to be used, layer thickness, ambient climate conditions (temperature, RH and indication of air speed) as function of time and whether the output is to be given as MC/CM or RH value. The user input will together with material data for the chosen material generate all the input data necessary for the computer simulations, see also chapter 5. After the simulations has finished the results will be presented in the user interface, for example as shown in Figures 5.1 and 5.2.

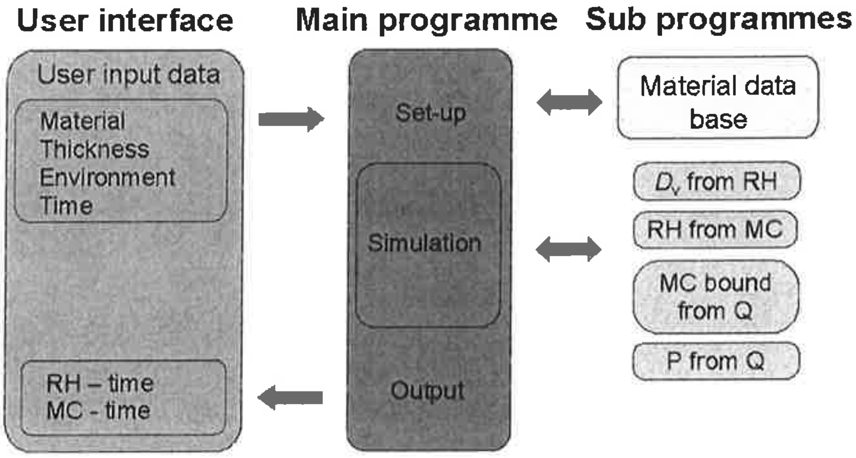

Figure 4.1: Schematic view of the structure of the programme.

Chapter 5

Description of programme modules

The programme is built up from one main programme and several sub-programmes, so called functions. The main program performs the simulations and calls upon the sub-programmes in order to obtain certain data as is further described below.

5.1 User input interface

In the user input interface the user will chose product, layer thickness and drying climate as a function of time. These data will together with the material data taken from the material data base make up the input data to the simulations. The user will also chose whether the result of the simulation should be presented as RH or MC values and when to end the simulation, after a certain time or when a certain moisture state is reached.

5.2 Material data base

Each material's data are stored in a separate file in the material data base. When the user selects a material the specific file is taken from the material data base and prepared for the simulations. Material data stored in each file are:

Moisture diffusion coefficient, D_v ($\mathrm{m^2s^{-1}}$), as a function of RH.
Moisture sorption, ($\mathrm{g\ m^{-3}}$), as a function of RH.
Heat developed, Q ($\mathrm{Jg^{-1}}$ dry mortar), at complete hydration.
Heat production rate, P ($\mathrm{Wg^{-1}}$ dry mortar), as a function of heat, Q.
Chemical binding of water, ($\mathrm{g\ m^{-3}}$), as a function of heat, Q.
Activation energy, E_a ($\mathrm{Jmol^{-1}K^{-1}}$).
Surface resistance ($\mathrm{s\ m^{-1}}$).
Density, ρ ($\mathrm{g\ m^{-3}}$).
Initial moisture content (amount of mixing water), ($\mathrm{g\ m^{-3}}$).

RH in material when hydration ceases, (-).

All data in this file are read and stored by a sub-programme, see section 5.3, when executing the programme.

5.3 Reading and storing input data

When a certain material and relevant climate conditions are chosen by the user, the data preparation sub-programme will read the specific material data file and user input data and store all data in the workspace, that is, make them accessible for the simulation programme.

5.4 Preparing data for simulation

This is a sub-programme that arranges all input data in suitable vectors for the main simulation programme. While preparing the data, the sub-programme will for example divide the material into cells as described in Figure 3.1, calculate the vapour pressure at saturation for the present temperature and set the start values for the simulation.

5.5 Chemically binding of water

This sub-programme calculates the amount of water that has been chemically bound in the material. The calculation is based on the heat produced which is proportional to the extent of reaction, see section 3.6. The thermal power, which is proportional to the rate of reaction, consequently describes the rate at which chemical binding of water occurs.

5.6 Determination of RH in material

The simulation programme generally uses the moisture content when simulating the moisture state of the material. However, some processes (moisture transport and rate of reaction) also need vapour content and relative humidity as potentials. The moisture content therefore needs to be translated into vapour content and RH. The present sub-programme uses the sorption isotherm to determine RH from the moisture content and by combining RH and temperature, the vapour content is determined.

5.7 Determination of reaction rate

The simulation programme calculates the heat (proportional to the extent of reaction). The heat is, together with the RH from section 5.6, and the current temperature, translated into the reaction rate. The reaction rate describes the development of the material regarding chemical binding of water and structure. The latter influences both moisture sorption and moisture transport, although this is not taken into consideration in the present version of the programme.

5.8 Determination of diffusion coefficient

This sub-programme calculates the diffusion coefficient from the RH in each cell.

5.9 Main simulation programme

The first part of the main programme describes the initial hours after casting, which are treated separately as described in section 3.3.

The second part and the heart of the main programme is built up in two loops. The inner loop calculates the development of the drying process and the related properties, see sections 3.4 - 3.9. The calculations are made in small time steps, see below. At certain time intervals, twice a day, the simulation enters the outer loop where data are saved and a new time step is calculated to optimize the calculation process. The time step depends on the diffusion coefficient, the moisture capacity (slope of the sorption isotherm) and the difference in moisture state between two adjacent cells. The moisture transport during a time step between two adjacent cells must never correspond to a value larger than half the difference in moisture content prior to the time step. In the present version this moisture transport corresponds at most to about 10% of the above described difference. In this outer loop it is also checked whether the simulation is finished or not. If not, the simulation enters the inner loop once again. If finished, the main programme enters it s third part where it calls upon the sub-programme Output, section 5.10, to organize and present the simulation data to the user.

5.10 Output

The sub-programme Output presents the results of the simulation to the user. The results can either be presented as relative humidity values, as shown in Figure 5.1 or moisture content values, as shown in Figure 5.2.

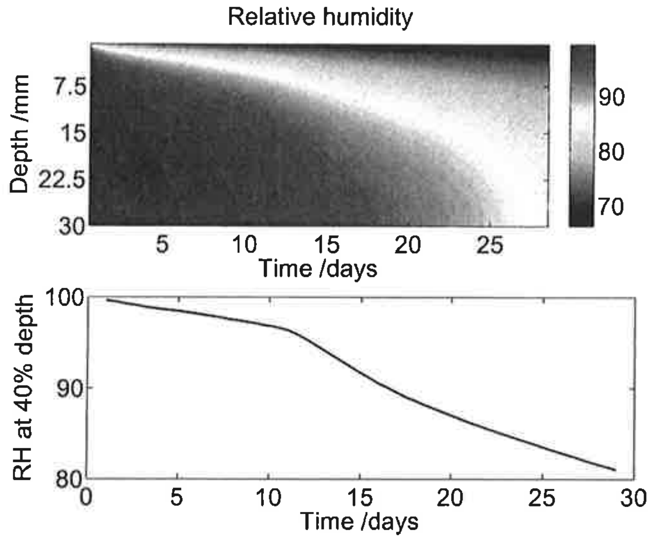

Figure 5.1: Example of results from a simulation under constant climate conditions. The results are presented as a relative humidity profile (top) and as relative humidity at 40% depth (bottom).

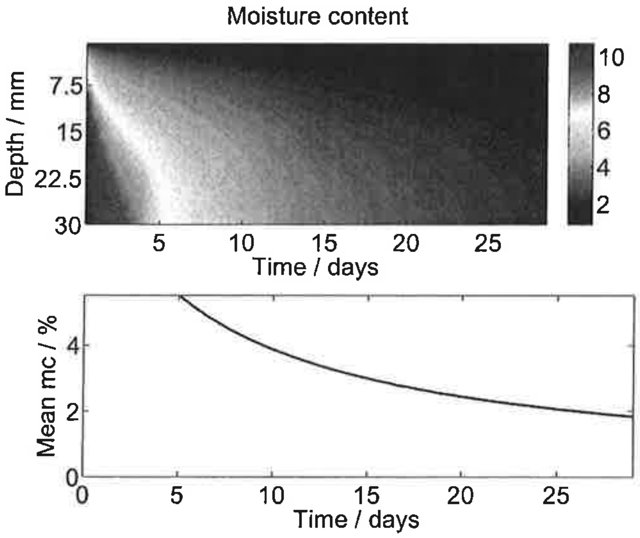

Figure 5.2: Example of results from a simulation performed under constant climate conditions. The results are presented as a moisture content profile (top) and mean moisture content (bottom).

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