Fungal Growth Prediction on Building Materials by Reaction-Diffusion Model Coupled with Heat and Moisture transfer

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Abstract
A mathematical model that reproduces fungal proliferation and morphological colony formation was developed on the basis of a reaction diffusion modeling approach. In this modeling, fungus was separated into two states, active and inactive, and it was assumed that active fungus moves by diffusion and reaction while generating and producing inactive fungus. The effects of temperature and humidity on fungal growth were explicitly incorporated in the reaction term of nutrient consumption/generation of active fungus in this governing equation. The damping function, which reproduces the effects of temperature and humidity on fungal growth, was developed and explicitly based on the fungal index proposed by Abe. In order to estimate the sensitivity of the proposed numerical fungal growth model, fungal growth on the surface of building materials was analyzed for four types of building materials, and the prediction results were compared with the results of WUFI-Bio.

Keywords: Fungi, Reaction diffusion model, Heat and moisture transfer, Indoor environment

Introduction

Fungal growth in indoor environments is strongly related to the indoor physical and chemical conditions, such as atmospheric temperature, relative humidity and nutrients; therefore, a comprehensive prediction method must be developed to estimate the health risk of fungal contamination for exposed individuals. Large numbers of studies have also shown an association between the health risk of fungal contamination and residence in homes with signs of ‘dampness’. Wickman et al. reported associations between damp houses and the presence of dust-bound micro-fungi in the homes of healthy children but not in the homes of atopic children (Wickman et al., 1992), and adverse effects on health due to micro-fungi exposure have become a serious problem.

The pollution problems caused by fungi in indoor environments are usually recognized at a stage where colony formation has progressed to a level enabling visual identification In other words, the prediction and control of the adverse effects of fungi on health at an early stage of fungal growth are usually difficult because of the lack of both prediction methods and detailed information regarding the effects of various indoor physical, chemical and biological parameters on the germination of spores and subsequent hyphal growth and colony formation.

In the field of mould/fungi growth prediction by computational simulation, WUFI-Bio is widely used to estimate spore germination and subsequent mould growth on building materials. WUFI is hygro-thermal calculation software developed at the *Fraunhofer Institut für Bauphysik*, Germany, and WUFI-Bio is an additional function of WUFI (add-on software) that was developed to estimate the probability of growth of some species on building surfaces.

This research focuses on the development of a simplified prediction model for two dimensional fungal growth in indoor environments, which incorporates heat and moisture transfer analysis in building materials.

Theory

Reaction diffusion model of fungal growth

In the present study, a mathematical model that reproduces fungal proliferation and morphological colony formation was developed on the basis of a reaction diffusion modeling approach. In this model, the fungus was hypothetically separated into two states, active and inactive. In this modeling, it was assumed that active fungus moves by diffusion and reaction while generating and producing inactive fungus at a constant rate. In terms of the morphology of colony formation, colonies might form a ring shape like a doughnut with the perimeter containing active fungus and the center containing inactive fungus. Concerning the inactive fungus, which is produced by the dynamism of the active fungus, neither extinction nor movement is considered and it is simply modeled as accumulating at the place it was generated.

Using these assumptions, a non-linear reaction diffusion model, which is coupled with temperature and humidity transfer in building materials, was adopted and is expressed by the following partial differential equations.

[1] The transport equation of active fungi, *u*

$$\frac{\partial u}{\partial t} = \nabla \cdot \left(D_c \nabla u\right) + \theta f\left(u,n\right) - a\left(u,n\right)u - \gamma u \quad (1)$$

$$D_c = \sigma_1^{'} \cdot u \cdot n\,,\quad \sigma_1^{'} = \sigma_1\left(1+\delta\right),\quad -0.5 < \delta < 0.5 \quad (2)$$

$$f\left(u,n\right) = \sigma_2\left(\frac{f_1 n}{1+f_2 n}\right) \cdot u \cdot \zeta\left(T,\varphi\right) \quad (3)$$

$$\zeta\left(T,\varphi\right) = a_1\,exp\left(a_2\varphi^2 + a_3T^2 + a_4\varphi * T + a_5\varphi + a_6T + a_7\right) \quad (4)$$

$$a\left(u,n\right) = \sigma_3 \cdot \frac{1}{\left(1+\frac{u}{a_1}\right)\cdot\left(1+\frac{n}{a_2}\right)} \quad (5)$$

[2] The transport equation of inactive fungi, *v*

$$\frac{\partial v}{\partial t} = a\left(u,n\right)u \quad (6)$$

[3] The transport equation of nutrients

$$\frac{\partial n}{\partial t} = D_n \nabla^2 n - f\left(u,n\right) \quad (7)$$

[4] The hygro-thermal transport equations

$$\frac{dH}{dT} \cdot \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + h_v \nabla \cdot \left(\delta_p \nabla (\varphi p_{sat}) \right) \tag{8}$$

$$\frac{dw}{d\varphi} \cdot \frac{\partial \varphi}{\partial t} = \nabla \cdot \left(D_\varphi \nabla \varphi + \delta_p \nabla (\varphi p_{sat}) \right) \tag{9}$$

Here, u and v are the hypothetical densities of active and inactive fungi, respectively. The total density of fungus is given by (u+v). n is the concentration of nutrients. The first term on the right side of equation (1) expresses the non-linear diffusion term that indicates the random movement of fungus. The second term is the reaction and generation term, which depends on the density of active fungus, nutrient concentration and other environmental factors. The third term refers to the conversion from active to inactive fungus and the fourth term expresses the rate of death of active fungus. The term on the right side of equation (6) expresses the generation of inactive fungus transformed from active fungus (same as the third term in equation (1)).

Equation (4) shows the damping function of fungal growth as a function of temperature T and relative humidity φ. In this study, the damping function $\zeta(T, \varphi)$ is expressed according to the fungal index proposed by Abe (Abe, 1993). This damping function is incorporated into the reaction and the term relating to the generation of active fungi, and the effect indirectly influences fungal diffusion.

Equation (7) shows the transport equation of nutrients and the first term on the right side of the equation indicates the diffusion of nutrients on the two-dimensional surface, and D_n is the diffusion coefficient of nutrients. The second term denotes the nutrient consumption by active fungus. Although it is thought that various types of nutrients influence fungal growth, nourishment of fungi was assumed in this study.

Equations (8) and (9) show the simultaneous heat and moisture transport and, here, dH/dT denotes the heat storage capacity of the moist building material, $dw/d\varphi$ denotes the moisture storage capacity of the building material, T is temperature and φ is relative humidity.

In the present study, for purposes of simplification, only nutrient concentration, temperature and relative humidity were focused on and these parameters non-homogeneously distributed on the surface of building materials were assumed to be the dominant environmental parameters in fungal growth.

Prediction of spore germination and mould growth by WUFI-Bio

WUFI-Bio was developed at the *Fraunhofer Institut für Bauphysik*, Germany, in order to describe non-steady fungal growth on the surface of building materials. The characteristic WUFI-Bio model is used to determine the moisture content within spores in order to predict bio-hygrothermal phenomena of spore germination and subsequent growth of hypha. The fungal growth rate in the WUFI-Bio model is calculated using isopleth diagrams, which were determined under constant temperature and humidity conditions. WUFI-Bio is a simulation model coupled with unsteady hygrothermal analysis of building materials and used worldwide.

In this study, the prediction results of WUFI-Bio were used to estimate the sensitivity of the reaction diffusion model.

Prediction of hypha growth by fungal index

Fungal index was proposed as a parameter to characterize the indoor environmental capacity for fungal growth and is widely used in Japan. This fungal index is based on the growth response of a xerophilic fungus *Eurotium herbariorum* as a function of ambient temperature and relative humidity. Fungal index is also based on isopleth diagrams under steady-state environmental conditions. The prediction results of fungal index were also used to evaluate the sensitivity of the reaction diffusion model.

Furthermore, in this research, fungal index was used as the damping function $\zeta(T, \varphi)$, which is expressed by equation (4) for the reaction diffusion model. In the condition that fungal index (mycelium length) is assumed to be a dependent variable and temperature and relative humidity are assumed as independent variables, the approximate expression $\zeta(T, \varphi)$ based on isopleth diagrams of fungal index was assumed using the non-linear and minimum-square approximation method. The parameters in equation (4) were a_1=1.089, a_2=-170.195, a_3=-0.012, a_4=-1.241, a_5=347.922, a_6=1.784 and a_7=-182.404 (R^2=0.929). In this approximation, $\zeta(T, \varphi)$ has the unit of mm/week.

Numerical Analysis

In this analysis, heat and moisture transfer and fungal growth on an indoor wall surface were analyzed for four building materials: (i) concrete single wall, (ii) gypsum plaster single wall, (iii) insulation board and (iv) composite wall consisting of (i), (ii), (iii) and an air layer, under summer climate conditions in Fukuoka, Japan. The building material of case (iv) is shown in Figure 1. Numerical analyses of heat and moisture transfer in building materials were carried out in one-dimension. Numerical predictions of fungal growth of (1) WUFI-Bio model, (2) fungal index proposed by Abe and (3) the reaction diffusion model proposed in this paper were conducted following temperature and relative humidity analyses on the surface of building materials.

Table 1 shows the cases analyzed and Table 2 shows the physical properties of the target building materials, which were obtained from the IBP database.

Concerning the case of the reaction diffusion model, its model parameters were identified using fundamental experimental data of colony formation and set by consideration of the results of previously conducted sensitivity analysis (see Ito and Mizuno, 2008). A two-dimensional plane of 200 mm (y) × 200 mm (z) on a wall surface (indoor side) was targeted as the object surface in this analysis. An equally spaced mesh with 1 mm intervals was adopted for the y and z directions for analysis of the reaction diffusion model. A uniform distribution of nutrient concentration was assumed as the initial condition. As the initial condition of active fungus, u = 1.0 was set at the center of the analytical plane (point x=100 mm and y=100 mm). The initial concentration of inactive fungus was assumed to be zero (v= 0.0). A free slip condition (zero gradient) was assumed as the boundary condition at the edge of the analytical plane. Each transport equation (eqs. (1), (6) and (7)) was discretized by the finite volume method, and unsteady analyses were carried out using the explicit method for solving time-variable partial differential equations. Calculations totaling 168 hours were conducted in real time. Table 3 shows a list of model parameters and other boundary conditions used for the numerical analysis. Stochastic fluctuation as shown in equation (2) was coupled in this analysis.

Results

Time course of temperature/relative humidity on the inner surface of building materials

Figure 2 depicts the time courses of temperature and relative humidity on the surface of target building materials (indoor side) and the outdoor climate conditions in summer. The calculation period covered was the first week of July in Fukuoka, Japan. The initial conditions of room air temperature and relative humidity were set at 25 ℃ and 85% RH, respectively, and the room air temperature and relative humidity were fixed at constant values. The heat and moisture transfer analyses were carried out at one hour intervals using WUFI software.

The outside temperature changed within the range of 19 ℃ - 32 ℃ on the basis of the AMeDAS data of a standard year. Wall surface temperature (indoor side) became constant at about 25 ℃ in cases (iii) insulation board and (iv) composite wall. In cases (i) concrete single wall and (ii) gypsum plaster single wall, although the wall surface temperature (indoor side) fluctuated, the temperature changes were smaller than the outdoor temperature fluctuation.

The outside relative humidity in this climate condition changed within the range of 50% RH – 100% RH on the basis of the AMeDAS data. Relative humidity on the wall surface (indoor side) became constant at about 85% RH in cases (iii) insulation board and (iv) composite wall. In the case of (ii) gypsum plaster single wall, relative humidity on the wall surface became relatively high.

Time course of hypha growth by numerical prediction

Figure 3 depicts the time course of fungal growth on each wall surface (indoor side). The prediction results of (1) the WUFI-Bio model overestimated the fungal growth response compared with the results of (2) fungal index. In the cases of (i) concrete wall and (ii) gypsum plaster board in particular, large differences were observed in the fungal growth response after 24 h from the start of analysis, although a difference in hyphal growth could not be confirmed at an earlier stage of analysis in (2) fungal index. For (2) fungal index, a high dependency of fungal growth on the target building materials was confirmed. In other words, the results of (2) fungal index had high sensitivity for the temperature and relative humidity compared with those of (1) the WUFI-Bio model.

The results of (3) the reaction diffusion model proposed in this study showed a similar pattern to the results of (1) the WUFI-Bio model.

Figure 4 shows the time course of colony formation predicted by the reaction diffusion model in Case3(II)g_S and Case3(IV)m_S. The morphological characteristics of the fungal colony were schematically predicted in modeling active and inactive fungi separately. In the early stage of calculation (less than 24 h), fungal colonies grew rapidly and seven days after the test started, the result of numerical analysis showed a tendency to increase constantly, but the amount of active fungus (*u*) did not appear to change markedly especially in Case3(IV)m_S. In this numerical analysis, the fluctuation of diffusion coefficient, which is expressed by Eq. (2), was coupled and then the phenomena of asymmetry and non-uniform diffusion were reproduced comparatively.

Discussion

There was a substantial difference between the prediction results of the WUFI-Bio model and the fungal index. This was caused by differences of the isopleth diagrams of growth response as a function of temperature and relative humidity. The WUFI-Bio model adopted more than 10 types of fungal growth response data. In comparison, fungal index was based on three types of fungi: *Eurotium herbariorum*, *Altermaria alternate* and *Aspergillus penicillioides*.

The prediction results of the reaction diffusion model were strongly dependent on the values of model parameters (σ_1, σ_2, f_1, f_2, θ, σ_3, a_1, a_2,) and nutrient condition (n_0, D_n). These model parameters were estimated heuristically to correspond to the results of the WUFI-Bio model in this analysis. The theoretical determination of these model parameters is a goal of future research.

Conclusions

The findings obtained in this work can be summarized as follows:

(1) Fungal index had a high sensitivity to temperature and relative humidity on the surface of building materials compared with the results of WUFI-Bio and the reaction diffusion model proposed in this study. From the viewpoint of predicted hypha length, the result of the WUFI-Bio model was the longest and the result of the reaction and diffusion model was similar to that of the WUFI-Bio model.

(2) The morphological characteristics of fungal colony formation could be reproduced on the basis of reaction diffusion expression in modeling active and inactive fungi separately.

(3) As the next step of this research, model parameters must be identified on the basis of detailed experimental data, and it is also necessary to couple numerical analysis with other parameters, for example characteristics of building materials and pH, in the proposed mathematical model.

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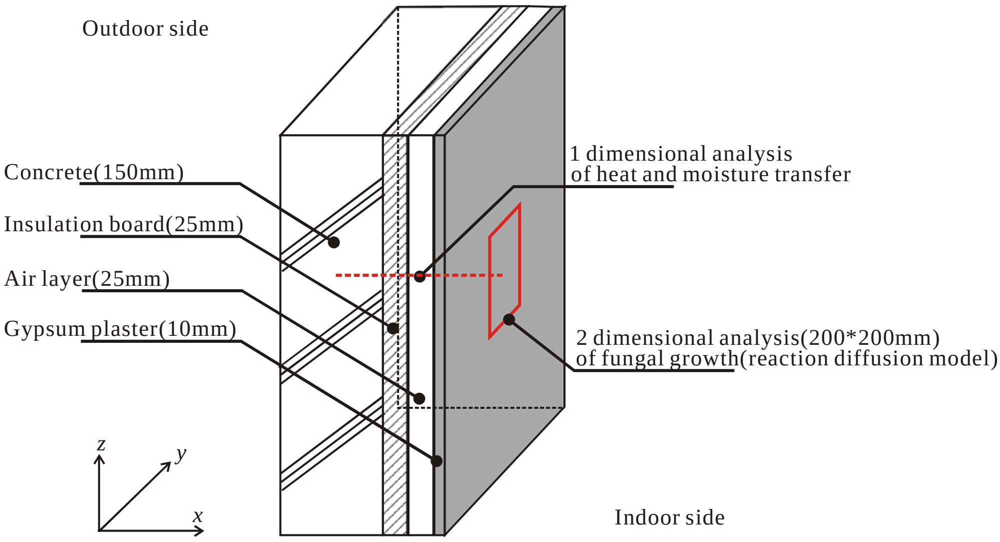


Figure 1 Target building materials (case (iv) composite wall)

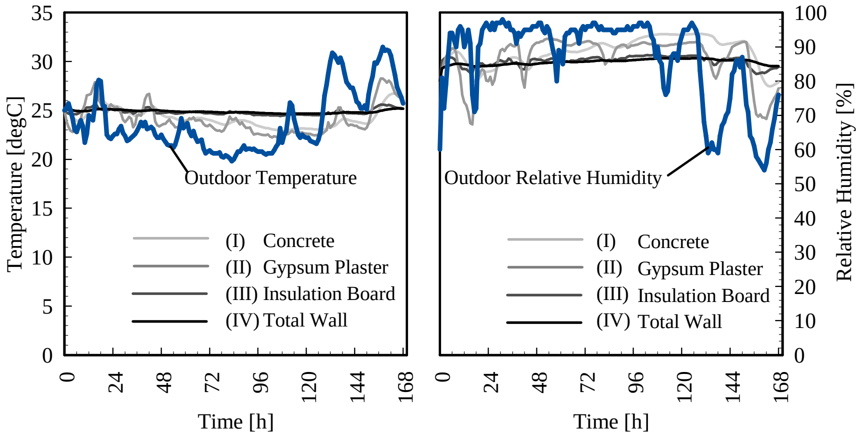
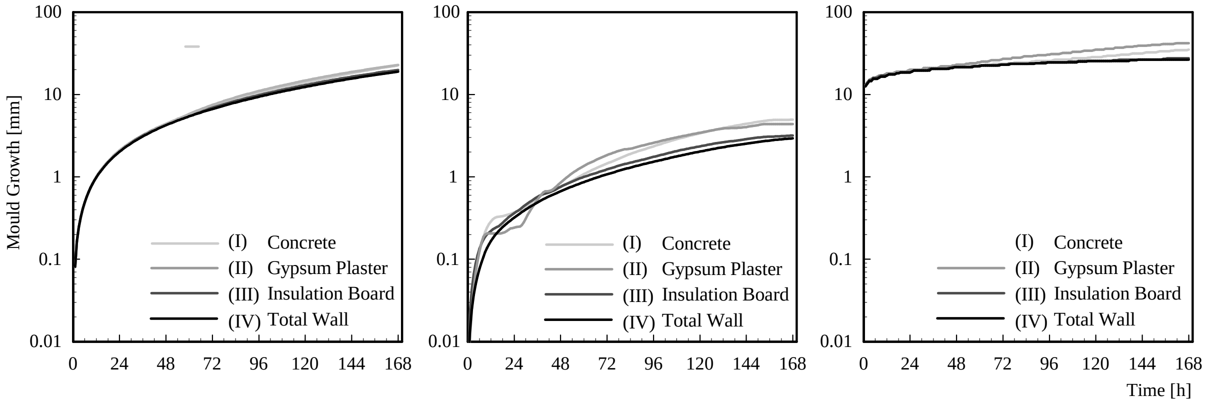
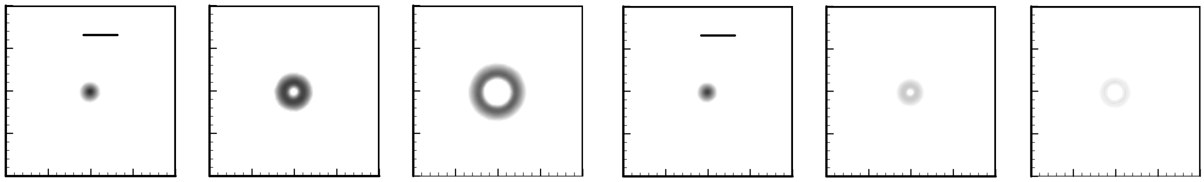


Figure 2 Results of time courses of temperature (left side) / relative humidity (right side fig.)



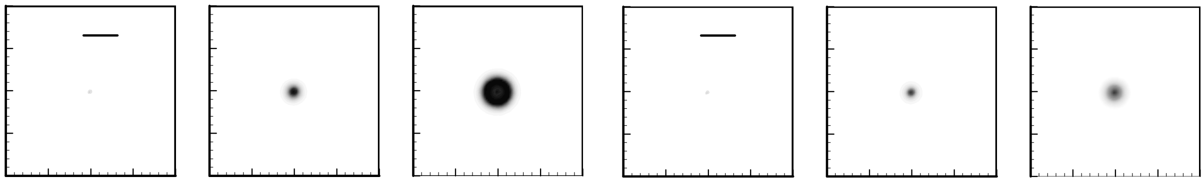
(1) Case 1 (WUFI-Bio) (2) Case 2 (Fungal index) (3) Case 3 (React. diff.)

Figure 3 Results of hypha length prediction [mm]



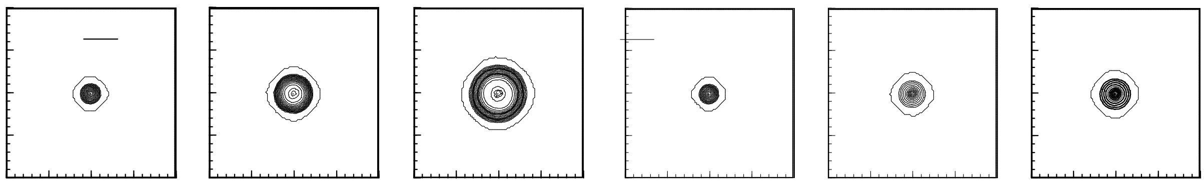
24h 96h 168h 24h 96h 168h

(1) Case3(II)g_S, Active fungi (*u*) (4) Case3(IV)m_S, Active fungi (*u*)



24h 96h 168h 24h 96h 168h

(2) Case3(II)g_S, Inactive fungi (*v*) (5) Case3(IV)m_S, Inactive (*v*)



24h 96h 168h 24h 96h 168h

(3) Case3(II)g_S, Active +Inactive (*u*+*v*) (6) Case3(IV)m_S, Active +Inactive (*u*+*v*)

Figure 4 Results of morphological characteristics of fungal colony formation

Table 1 Cases analyzed

	(I) Concrete (150^{mm})	(II) Gypsum plaster (10^{mm})	(III) Insulation board (25^{mm})	(IV) Composite wall ((i)+(ii)+(iii)+air layer) (210^{mm})
(1) WUFI-Bio	Case 1(I)c_S	Case 1(II)g_S	Case 1(III)a_S	Case 1(IV)m_S
(2) Fungal index	Case 2(I)c_S	Case 2(II)g_S	Case 2(III)a_S	Case 2(IV)m_S
(3) React. diff. model	Case 3(I)c_S	Case 3(II)g_S	Case 3(III)a_S	Case 3(IV)m_S

Table 2 Physical properties of target building materials

Material	Thickness [mm]	Bulk density [kg/m^3]	Porosity [m^3/m^3]	Specific Heat Capacity (dry) [J/kgK]	Thermal Conductivity (dry) [W/mK]	Water Vapor Diffusion Resistance Factor [-]
(I) Concrete	150	2200	0.18	850	1.6	92
(II) Gypsum Plaster	10	1721	0.305	850	0.2	13
(III)Insulation Board	25	28.6	0.99	1470	0.025	170.56

Table 3 Numerical and boundary conditions

Calculation period	Total 168h, Time Steps:1[h], Start:07/01, End:07/09
Initial Condition (wall inside)	Initial Temperature[℃] : 25 ℃, Initial Relative Humidity[-] : 0.6 Initial Water Content[kg/m^3] of Concrete: 41.3, Insulation Board : 0.16, Gypsum Plaster : 1.13
Indoor Climate	Temperature[℃] : 25℃ constant, Relative Humidity[-] : 0.85 constant
Outdoor Climate	Fukuoka; AMeDAS standard year (07/01 to 07/09)
Model parameters of Reaction diffusion model	σ_1=5.0×10^{-5}, σ_2=3.0, f_1=1.0, f_2=1.0,θ=5.0×10^2, σ_3=5.0, a_1=1/2400, a_2=1/120, n_0=1.0 for PDA, D_n=1.0×10^{-9}, u_0 (center)=1.0, v_0=0.0