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Combining three main modeling methodologies for heat, air, moisture and pollution modeling

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Abstract

In the paper we consider three types of numerical simulation tools: Finite Element Method (FEM), Building Energy Simulation (BES) and State-Space (SS) together for Heat, Air, Moisture and Pollution (HAMP) modeling. We developed a simplified reference model regarding a residential building zone, for benchmarking the three mentioned modeling methodologies, i.e. BES, FEM, SS, including, Heat, Air, Moisture and Pollution (HAMP) physics. BES is based on lumped parameter modeling. By using FEM, the BES results can be extended to 3D high resolution images. Furthermore, by using SS, the computing time can be drastically reduced in order to make optimization of operation strategies possible. It is concluded that the main benefits of FEM-SS-BES modeling exchange is the possibility to simulate building energy performances with high spatial resolution and low computational duration times.

Keywords: heat, air, moisture, pollution, modeling, methodology

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1. Introduction

Highly energy efficient residential buildings need to be rather airtight, and they will include systems to ensure that the need for ventilation is met in an optimal way. Achieving such energy optimized performance can encompass a risk of high levels of pollutants indoors: Humidity, particles and various chemical compounds, where the first and the latter can both be absorbed by and emitted from materials in the building fabric and furnishings. The IEA EBC Annex 68 project "Indoor Air Quality Design and Control in Low Energy Residential Buildings" [1] will gather the existing

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scientific knowledge and data on pollution sources in buildings, models on indoor hygrothermal and air quality as well as thermal systems, and will look to ways to optimize the provision of ventilation and air-conditioning. One of the key objectives is to develop tools for building operation strategies regarding ventilation and its control, thermal and moisture control and air purification strategies - and their optimal combination. An overall objective of energy efficiency in the built environment is to improve building and systems performances in terms of durability, comfort and economics. In order to predict, improve and meet a certain set of performance requirements related to the indoor climate of buildings and the associated energy demand, numerical simulation tools are indispensable. In this paper we consider three types of numerical simulation tools: Finite Element Method (FEM), Building Energy Simulation (BES) and State-Space (SS). For each tool separately, there exist a vast number of references. Also on two tools combined, i.e. FEM-BES, BES-SS, FEM-SS, there is quite a lot of literature. However there is lack of research on an overall evaluation of the three tools FEM-SS-BES together. In this paper we present benefits of the FEM-SS-BES modeling exchange for building physics. The main reasons for converting models in each other are summarized in Table 1.

Table 1. The main reasons for converting models in each other

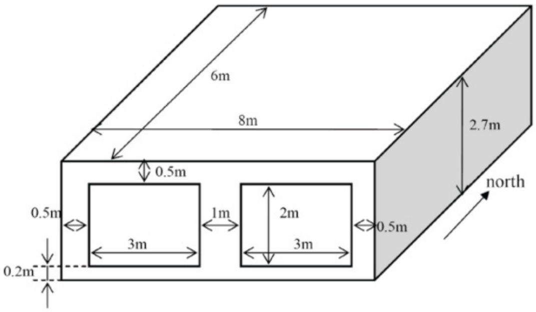
To From	FEM	BES	SS
FEM	*	Global effects Lumped results	Computation Speed
BES	Local effects High resolution results	*	
SS		Inverse Modeling	*

In this work FEM is just a method of solving Partial Differential Equations (PDEs), like Finite Volume methods (FVM) or Finite Difference methods (FDM). We start with two combinations that are quite obvious and already commonly used. *BES to FEM* – BES is used to simulate the energy performance of buildings, using lumped parameter modeling. If local effects are important, FEM can be used to obtain high resolution results based on distributed parameter models and using BES simulation results as boundary values. *FEM to SS* – FEM based simulations can easily become computational time consuming. One of the methods to improve the computing time is to reduce the mathematical model to a lower order model by using for example a State-Space (SS) approximation. One of the main benefits of SS models is, that very efficient computation algorithms exist, that are able to almost completely reduce the computation time. If such a reduced order SS model is accurate enough, this method can be used for improving computation speed. Previous work on FEM-SS-BES modeling is shown in [2]. So far the FEM-SS-BES modeling is focused on single physics (heat transfer). In this paper we present a FEM-SS-BES model for a multiphysics application, namely the integrated heat, air, moisture and pollution simulation of simple room. The main application is a combined heat, air, moisture, pollutant (HAMP) SS model verified with a BES model. One of the key objectives is to develop tools for building operation strategies regarding ventilation and its control, thermal and moisture control and air purification strategies and their optimal combination, see also [1]. If pollutant absorption and desorption of walls is neglectable, HAMBase can be used as a tool for optimizing the control and operation strategy. However due to the large amount of simulations that are necessary for optimization studies, HAMBase could be impractical to use. In this case the very time-efficient SS model can be used also including the possibility of pollutant adsorption and desorption of walls. Section 2 provides the modeling, Section 3 the simulation results and Section 4 presents the conclusions.

2. Modeling

2.1. BES Model

The BES model is based on a simplified BEStest building [3]. Fig.1, left shows the geometry. The simplified model consists of: one zone; one wall including one window; one source for heat, moisture and pollutant each; a constant ventilation. The external climate is a typical Dutch year. The main characteristics are provided in Fig. 2, right.



Simplified BEStest building, Free Floating for HAMP

Dimensions: 4m x 3m x 5m

One wall: 3m x 4m (10cm brick; 10cm EPS; 10 cm brick)

One floor: 4m x 5m (10 cm brick; 20 cm EPS)

One window: 1m x 2m (Uvalue 1.3 W/m^{2}K)

Air ventilation: 1/hr (constant)

On/off profile all sources: 1 between 8:00 – 18:00, 0 elsewhere

- Heat source: 200W
- Moisture source: 55 mg/s
- Pollutant source: 55 mg/s

Fig.1. Left: The geometry of the BEStest building; Right: The parameters of the simplified BEStest building

The model is implemented in HAMBase [4]. A review paper including validation studies of HAMBase is presented in [5]. A recent application is provided by [6]. These studies do not include pollutant modeling. However, HAMBase facilitates the modeling and simulation of pollutants in air similar to vapor concentration, but without absorption of the walls. A verification study where HAMBase was used for simulating pollutant concentrations can be found in [7]. The simulation results of the HAMBase model of figure 1 is presented in Section 3.

2.2. SS Model

This Section presents the State-Space (SS) modeling development. The work of [8] already provides a validated state-space model for the heat and moisture transport in a single zone. Fig. 2, shows the model in the form of ordinary differential equations (ODEs). We used **x** as state and xdot as d**x**/dt. The first 5 states x(1) .. x(5) and time derivatives xdot(1) .. xdot(5) are identical from the model of [8]. Due to the expected symmetry in mass transport between vapor and pollutant, the states and accompanying time derivatives concerning the pollutant transport are similar to vapor transport. Thus defining x(6), x(7), xdot(6) and xdot(7).

```
x(1)=T1   xdot(1)=( -(x(1)- Te)/RT12   + (x(2)-x(1))/RT12                              )/CT1;
x(2)=T2   xdot(2)=( -(x(2)- Te)/RTvent - (x(2)-x(1))/RT12 -(x(2)-x(3))/RTsurf + STair  )/CT2;
x(3)=T3   xdot(3)=(                                       +(x(2)-x(3))/RTsurf + STsurf )/CT3;
x(4)=P4   xdot(4)=( -(x(4)- Pe)/RPvent                    -(x(4)-x(5))/RPsurf + SPair  )/CP4;
x(5)=P5   xdot(5)=(                                       +(x(4)-x(5))/RPsurf          )/CP5;
x(6)=w6   xdot(6)=( -(x(6)- we)/Rwvent                    -(x(6)-x(7))/Rwsurf + Swair  )/Cw6;
x(7)=w7   xdot(7)=(                                       +(x(6)-x(7))/Rwsurf          )/Cw7;
```

Fig. 2. The model in the form of ordinary differential equations (ODEs) code.

Explanation of the model of Fig. 2: The first letter(s) of each variable has the following meaning: x is the state, xdot is the time derivative of x, T is temperature; P is vapor pressure; w is pollutant concentration [kg/m^3]; R is resistance; C is capacity; S is Source;

The labels represent: 1 is center of the wall; 2, 4, 6 are indoor air; 3, 5, 7 are inside floor surface; e is external; vent is ventilation; surf is (floor) surface; 12 is the center of the wall.

The main reasons to present the model as shown in figure 2 are twofold:

Firstly, the symmetry between the main transport mechanism (heat, vapor and pollutant) is clearly visible. One can see that vapor and pollutant transport can be treated as the same, and heat transport is almost the same except: (a) one extra state for the temperature the wall (center), i.e. x(1) and xdot(1); and (b) and extra heat source at the inner surface representing the incoming irradiance through the window to the floor, i.e. the STsurf term at xdot(3).

Secondly, the model code of figure 2 can be directly implemented in scientific software such as Matlab but also for example Python. This may encourage modelers to implement the code into tools for integrated heat, air, moisture and pollutant (HAMP) transport. The latter is important for the key objectives of the current IEA EBC Annex 68 Indoor Air Quality Design and Control in Low Energy Residential Buildings [1]. In order complete the model, numerical values of all parameters are shown in Fig. 3. The results are shown in Section 3.

Constants

```
V=3*4*5;             % Volume [m3]
Vdot=3*4*5/3600;     % Airflow rate [m3/s]
rho_air=1.2;         % air density [kg/m3]
c_air=1000;          % specific heat [J/kgK]
Rc=2.8;      % Rc value construction [m2K/W]
Ac=3*4;      % Surface construction [m2]
Aw=1*2;      % Surface window [m2]
Am=5*4;      % Surface inside thermal material [m2]
hT=10;       % Surface heat transfer coefficient
hP=3e-8;     % Surface vapor transfer coefficient
hw=3e-3;     % Surface VOC transfer coefficient
fw=1e-4;     % Fraction = mass VOC / mass air
Rv=402;      % Gas constant for vapor
Tvref=283;   % T ref for Rv [K]
fCT=1e5;     % factor of thermal capacity comp. to air
fCP=5;       % factor of vapor capacity comp. to air
fCw=0.01;    % factor of VOC capacity comp. to air
we= 0       %Ext.VOC concentration [kg/m3]
```

```
RTvent=1/(4*Vdot*rho_air*c_air);
RPvent=Rv*Tvref/Vdot;
Rwvent=1/Vdot;
RT12=0.05*Rc/Ac;
RTsurf=1/(hT*Am);
RPsurf=1/(hP*Am);
Rwsurf=1/(hw*Am);
CT1=0.2*Ac*1500*840;
CT2=V*rho_air*c_air;
CT3=fCT*CT2;
CP4=V/(Rv*Tvref);
CP5=fCP*CP4;
Cw6=V;
Cw7=fCw*Cw6;

Te     %Ext. Temperature [oC]
STair  %heat source to air [W]
STsurf %heat source to surface [W/m2]
Pve    %Ext. vapor pressure [Pa]
SPair  %Vapor source to air [kg/s]
Swair  %VOC source to air [kg/s]
```

Fig. 3. The complete set of the model constants, parameters and the time dependent inputs

3. Simulation Results

3.1. BES-FEM Heat Air (HA) modeling verification

The heat and air transport of the BEStest building [3] was modeled and verified using Comsol [9] with satisfactory results, see Fig 4.

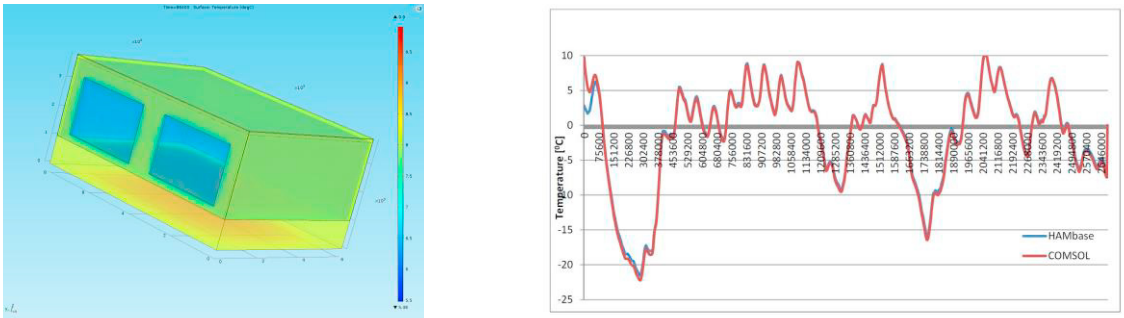


Fig. 4. Left: The BEStest building simulated using FEM (Comsol); Right: The simulated indoor temperature of BEStest benchmark 900FF using BES (blue) and FEM (red)

In Fig.4, left, a snapshot of the FEM simulation is shown. The high-resolution details are visible. Fig. 4, right, presents the simulated indoor mean temperature using FEM (Comsol) and BES (HAMBase) for a typical BEStest benchmark 900FF representing a free floating BEStest building with a heavy weight construction. As can been seen the temperatures of the BES and FEM are almost identical, indicating a very good verification for both models regarding the heat transfer. This paper focuses on the BES-SS HAMP modeling and the FEM modeling including moisture and pollutant transport is left over for future research.

3.2. BES-SS Heat Air Moisture Pollutant (HAMP) modeling verification

In Fig. 4, the simulated indoor air temperature, relative humidity and pollutant concentration of the two models BES (HAMBase, see Section 2.1) and SS (see Section 2.2) are presented.

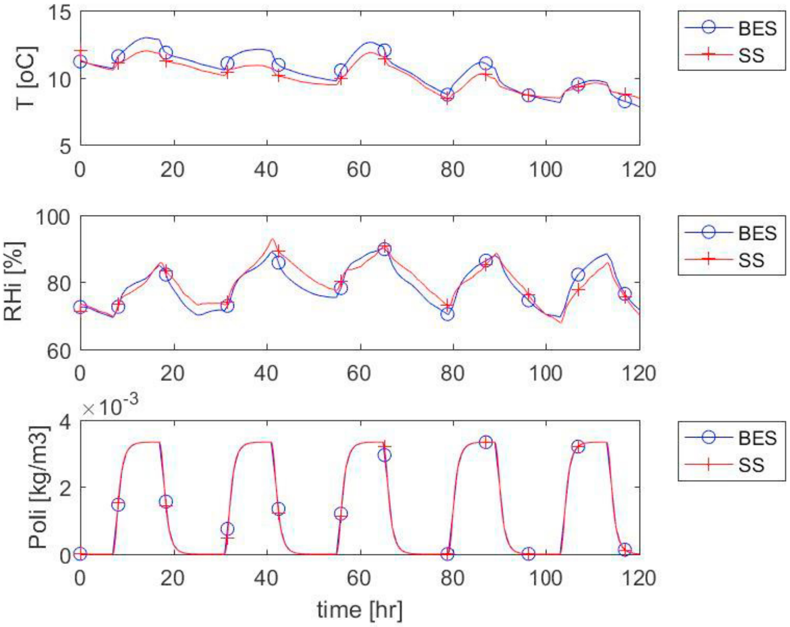


Fig. 4. The simulated indoor air temperature, relative humidity and pollutant concentration of the two models BES (blue) and SS (red) during simulation period of 5 days

In Fig. 4, top, the simulated free floating indoor air temperatures of the BES and SS models for 5 days using a typical Dutch climate are presented. Although the dynamics of both temperatures are similar, an improvement by optimizing some SS model parameters is expected to increase the correlation for verification purposes. The comparison of the relative humidities is shown in Fig. 4, middle. The results are somewhat better than the temperatures. Also here an improvement seems to be necessary for verification. Fig. 4, bottom, presents the pollutant concentrations. The results are almost identical, thus providing a verification for the pollutant transport for the BES and SS models. To summarize: The SS model seems to be accurate enough for further HAMP simulation tool development, however the verification for the heat and vapor transport still needs some attention to complete.

4. Conclusions

One of the key objectives of the current IEA EBC Annex 68 project “Indoor Air Quality Design and Control in Low Energy Residential Buildings” is to develop tools for building operation strategies regarding ventilation, control and air purification strategies. To do so, integrated heat, air, moisture and pollutant (iHAMP) models that are able to simulate the indoor climate are required. In this paper we presented three types of iHAMP models: Finite Element Method (FEM), Building Energy Simulation (BES) and State-Space (SS).

FEM: The heat and air transport of the BEStest building was modeled and verified using Comsol with satisfactory results. *Future work* is to include moisture and pollutant transport. The latter will be done in the framework of the IEA EBC Annex 68.

BES: HAMBase was used as BES model, based on a simplified BEStest building. HAMBase is capable of simulating iHAMP models with currently one limitation: The absorption and desorption of pollutants at surfaces is not included yet. The heat and moisture transfer of HAMBase was successfully verified by the Comsol model. A verification study of HAMBase by a State-Space model for heat, air, moisture and pollutant simulation is included in this paper. The conclusion are presented below.

SS: The main focus of this paper is the development of State-Space (SS) model for iHAMP. The model equations and all parameters are provided, allowing tool developers to implement this model into their software environments. The SS model was verified using HAMBase. The verification is not fully satisfactory yet. *Future work* is to optimize some SS model parameters, an improvement of the correlation is expected. The SS model seems to be accurate enough for further HAMP simulation tool development.

The reader should notice that the modeling type BES can have any level of complexity and all FEM and SS models in this paper can also be regarded as BES models. In this work BES models are represented by software such as HAMBase, Energy Plus, DOE, etc.

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