COUPLING STRATEGIES FOR COMBINED SIMULATION USING MULTIZONE AND BUILDING ENVELOPE MODELS

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ABSTRACT

Combined heat, air, moisture and pollutant simulations (CHAMPS) at the building system level are essential for improving energy efficiency and indoor environmental quality. This paper discusses the technical challenges and possible solutions to the problem of coupling an envelope model (CHAMS-BES) with a multizone/network model for inter-zonal air and pollutant transport. A representative multizone solver was written, which solves the coupled heat, air, moisture and pollutant transport equations. Several different methods for coupling this representative CHAMPS-multizone code with the CHAMPS-BES code were investigated. The implementation details of these solutions are presented and evaluated with respect to numerical performance, stability and flexibility. A recommended implementation is shown, which allows flexible coupling of different independent simulation codes, while providing an acceptable numerical accuracy.

KEYWORDS

Heat, air, mousture and pollutant transport; Modeling; Simulations; and Coupling.

INTRODUCTION

An integrated simulation environment for building system design and control requires not only robust and efficient component models for the building envelope, HVAC system, rooms and multizone heat, air, moisture and pollutant transport, but also efficienct coupling among these component models (Fig. 1). For energy performance simulation, methods for the coupling between a thermal model (including envelope and zone air) and a multizone network flow model, and the coupling between the thermal model and a CFD room model have been developed (e.g., Hensen 1991, Beausoleil-Morrison 2000, and Gu 2006), and have been implemented in some popular simulation tools such as EnergyPlus, ESP-r, TRANSYS, and DeST (Crawly et al. 2005). The coupling between multizone and CFD models have also been explored recently (e.g., Wang and Chen 2007 and Khalifa et al. 2007). However, the issue of coupling between the component models for combined heat, air, moisture and pollutant transport simulations remains to be fully investigated (Zhang 2005). This paper provides a systematic analysis of the possible approaches for the coupling between the Envelope and Multizone component models.

Current simulation codes for multi-zone air flow models typically do not include detailed models of building components that are part of the building envelope (e.g. walls, ceilings, floors, roofs etc.). Also source and sink characteristics of such components, particularly important for pollutant adsorption and emissions, can only be considered in a pre-prescribed and approximate manner. Consequently the effects of heat, moisture and pollutant storage and transport in building components on the air quality modeled in multi-zone models cannot be accurately calculated and predicted, while such effects could be significant, for example, in the evaluation of volatile organic compunds (VOCs) emissins and outdoor-to-indoor pollutant transport.

Tools for building envelope systems (e.g., CHAMPS-BES 2006) allow detailed calculation and prediction

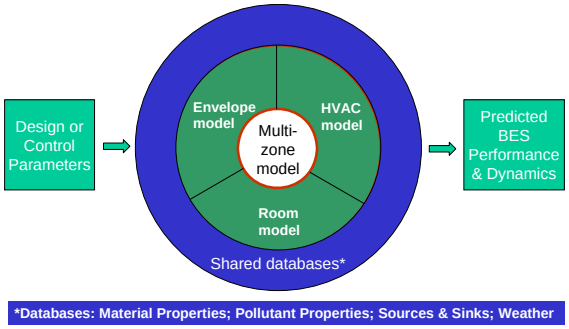

Fig. 1 A System Model for CHAMPS (Zhang 2005)

of transport and storage processes inside building components or building envelope systems (BES). However, their application is typically limited to the building component itself, for instance a wall-window interface or simply a multilayered wall or roof. The boundary conditions that affect the temperature, moisture and pollutant distributions inside the structures are dictated by outside climate and an assumed indoor climate. Transport processes over the boundary of building components would normally affect the indoor climate as well as the transport inside the building components, but cannot be calculated in current CHAMPS-BES models.

Coupling an Envelope and Multi-zone model in a combined simulation would allow the investigation

of coupled phenomena when needed, such as: (1) long term VOC emissions from assemblies of building materials and their effect on the indoor air quality (IAQ) for given HVAC design conditions; (2) moisture buffering effects and improved prediction of surface moisture conditions; and (3) thermal storage effects and improved prediction of surface temperatures.

GOVERNING EQUATIONS

To describe the air, heat, moisture and pollutant transport, the balance equations for each quantity have to be solved for each zone and inside each building component. In addition, flux densities across interfaces have to be modeled. The governing equations for either component models are the balance equations for the energy, air/gas mass, moisture mass (liquid water and water vapor) and a VOC/pollutant mass. These quantities can be summarized in the vector

$$\mathbf{E} = \{U, m_a, m_{w+v}, m_{VOC}\} \tag{1}$$

and the general mass conservation equation can be written as

$$\frac{\partial \rho^{<E>}}{\partial t} = -\frac{\partial}{\partial x_k} \sum j_k^{<E>} \tag{2}$$

where, ρ, t, x, k, and j represent density, time, coordinate, directions, and flux, respectively. $<E>$ indicates one component of the quantity vector **E**: internal energy U, air mass m_a, moisture mass m_{w+v} or pollutant/VOC mass m_{VOC}. These balance equations are the same in format for the multizone and envelope model, but in the envelope model a spatial distribution of these quantities is calculated, whereas in the multizone models the perfectly mixed quantities in each zone are balanced. Also, the calculation of the flux terms is different. In the envelope model, internal fluxes and boundary fluxes are calculated, while the balances for the multizone models only involve boundary fluxes and source and sink terms (Nicolai et al. 2007 and Zhang 2005).

Solution of air mass balance

For the multizone model, the air mass balance is solved as a steady-state equation, and reads for a single zone

$$0 = \sum_b q_b^{m_a} \tag{3}$$

where $q_b^{m_a}$ is the mass flow across each boundary or zone interface driven by pressure differences Δp_g. For instance, a typical flow model for a leakage path gives the flow rate as non-linear function of the pressure difference

$$q_b^{m_a} = C\rho\left(\Delta p_g\right)^n \tag{4}$$

where C and n are empirical parameters. Inside the envelope model, the air flow field is also calculated using a quasi steady-state flow equation, however, the pressure gradient is the driving potential:

$$0 = \frac{\partial}{\partial x_k}\left(-K_g \frac{\partial p_g}{\partial x_k}\right) \tag{5}$$

Depending on the material permeability K_g and boundary pressures a flow field is calculated. Details about the calculation algorithm can be found in (Grunewald et al. 2007).

Envelope–zone air interface conditions

For the envelope model, the important indoor boundary conditions are convective heat, water vapor and pollutant mass transfer through the boundary layer and radiation over the interior surfaces, and the advective transport of energy, vapor, pollutants via airflows across the zone interfaces. Various methods exist to model these processes as function of the surface conditions of the building component and the conditions in the adjacent zone. Using appropriate models for each quantity a flux density can be formulated (Zhang 2005).

These fluxes describe the exchange of conserved quantities (energy and masses) between the envelope component and multizone models, and must be consistently described in both models in order to obtain a combined model where mass and energy is conserved. They include:

- total heat flux in J/m^2s (energy balance equation)
- total enthalpy flux in J/m^2s (energy balance equation)
- total moisture/vapour flux in kg/m^2s (moisture mass balance equation)
- total VOC/pollutant flux in kg/m^2s (VOC/pollutant mass balance equation)

These total quantities combine convective and advective fluxes. For the convetive flux quantities, the following equations are used.

$j^U = -\alpha\left(T_e - T_b\right)$ convective heat transfer

$j^{m_v} = -\beta\left(p_{v,e} - p_{v,b}\right)$ convective mass transfer for water vapor

$j^{m_{VOC}} = -\gamma\left(c_e - c_b\right)$ convective VOC mass transfer

Note that for pollutant/VOC mass transfer, the mass concentration in kg/kg is used. The parameters α, β and γ are the surface mass transfer coefficients. The

mass and energy boundary fluxes are described within the multizone and envelope model using the same equations to ensure mass and energy conservation.

NUMERICAL INTEGRATION

As briefly shown in the previous section, the multizone model with discrete zones and envelope model are formulated mathematically as coupled systems of partial differential equations (PDE). Using the control volume technique, these PDEs can be transformed into sets of ordinary differential equations (ODE). For each zone in the multizone model a set of coupled ODEs is obtained, with one unknown per balance equation. The spatial discretization of the envelope model however, results in several interconnected elements, each with a set of coupled ODEs and unknowns.

The resulting system of equations needs to be numerically integrated in time. It has to be noted that the system functions are non-linear functions of the system variables. Considering the numerical solution of each model separately, it is beneficial to use a fully implicit method for the time integration (implying several iterations per time step), because of its stability properties. Also, some form of Newton iteration is recommended to improve the convergence properties of the scheme. While the details of numerical integration methods can be found elsewhere (e.g., Dols et al. 2000 and Nicolai et al. 2007), the specific method used in the representative multizone code and the CHAMPS-BES code developed in this study is briefly described in the following section.

Numerical integration of the multizone equations

For multizone models that solve the air mass balance equation for coupled zones, each time integration step typically requires several iterations, because of the coupling of the air pressures to the temperature distribution and non-linear permeability/connectivity functions. Also, the convective heat and mass transfer terms in the multizone model, considering moisture and pollutant convection, require iterative solution. While explicit methods are also possible, their poor stability properties typically require very small time steps. An iterative solution scheme ais adopted in this study as in many existing multizone simulation codes (Wang et al. 1998).

Numerical integration of the envelope equations

The tightly coupled heat and moisture balance equations require special consideration for the numerical integration in solving the envelope model. In the CHAMPS-BES code, a fully implicit Newton method is used. It is a variable-step, multi-step method that is very efficient, particularly for the highly non-linear transport and storage coefficients appearing in typical envelope simulation problems. The air flow field is calculated decoupled, as quasi-steady flow field and thus the air mass balance is not included in the integration scheme. The size of the integration steps depends on the history of the solution variables as well as the current derivatives of the system variables and is flexibly adjusted. Details on the solution method can be found in Hindmarsh et al. (2005) and Nicolai and Grunewald (2007).

ANALYSES OF COUPLING METHODS

Evaluation criteria and reference for comparisons

Considering a separately working multizone and envelope codes, and thus independent models, the effectiveness of the coupling algorithm can be evaluated based on:

- Accuracy: Clearly, solving the equations for the multizone and envelope models together and fully coupled will give an accurate solution within the tolerances of the numerical scheme. This solution is hence used as the reference against which solutions obtained with other coupling methods are compared against.
- Simulation time: The performance of the combined simulation environment is also critical. Ideally, the simulation time for the fully coupled multizone and envelop models would be only as long as the sum of the simulation time needed for integrating each model separately. The coupling schemes can thus be evaluated with respect to this ideal calculation time.
- Flexibility: The flexibility of the coupling is important. If one code needs to fully include another code, this will result in very inflexible software. Changes in one code will ultimately require changes in the other as well. In an optimal case each model and code can be developed independently, that means neither code needs to know about the structure, integration method or data organization of the other, while only knowing about a small and well defined interface module.

Classification based on mass/energy conservation

Many different possibilities exist to couple a multizone model and an envelope model in a combined simulation. In general, these methods can be either mass/energy conservative or non-conservative. In the former, mass and energy conservation become a convergence criterion during the integration, while this is not enforced in the later. In each category, the coupling methods can be further classified based on time-step control (Fig. 2).

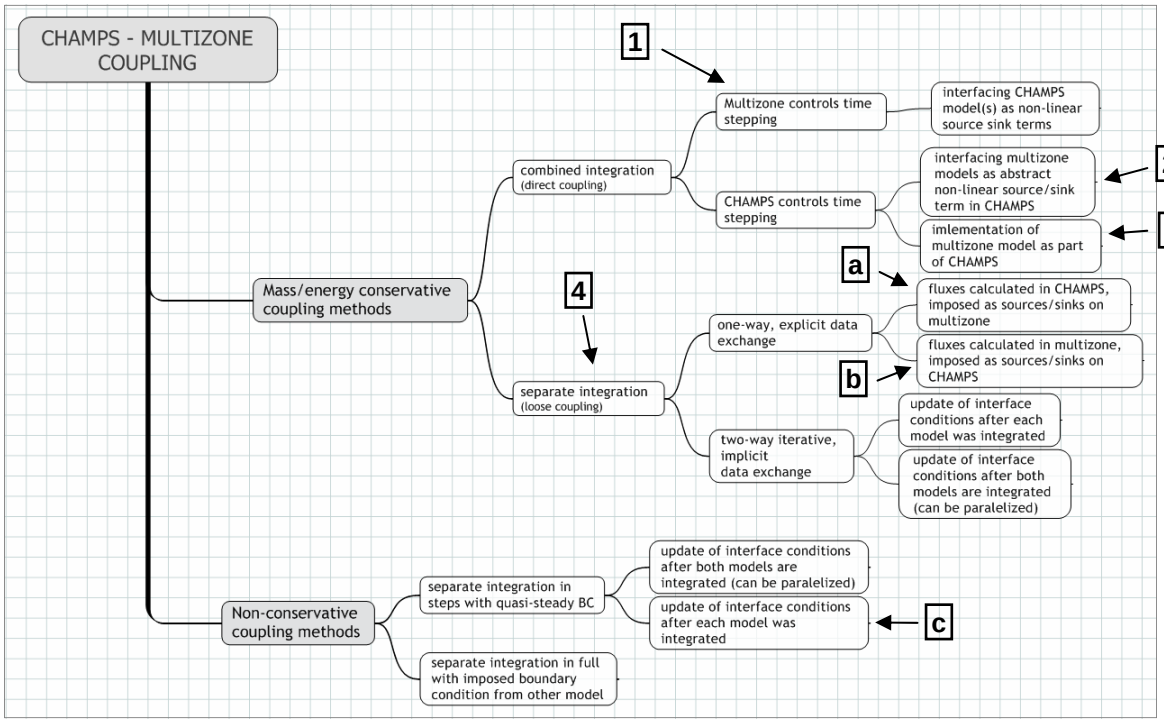

Fig. 2 Overview of possible methods for combined multizone and envelope simulation

For a conservative method the boundary/interface flux quantities presented in the previous section need to be consistently used in the multizone and envelope model. In order to achieve this, the calculation of the interface fluxes (that allow exchange of quantities between a zone element in the multizone model and the interfacing elements in the envelope model) should be done once for each interface and then the same flux quantity should be used for the integration of both models. The time integration of both models must ensure that the total mass and energy is conserved at the end of each time step (Fig. 2):

- Combined integration (direct coupling): The multizone and envelope balance equation systems are solved simultaneously in a *combined simulation*. The core simulation program can be either the solver of the multizone or envelope codes. The other model is then used as a component or directly integrated into the equation system.
- Separate integration (loose coupling): The two models are *integrated separately*, but synchronized at appropriate time intervals. Synchronization here means exchange of interface conditions information (e.g. zone temperatures, relative humidity, concentrations, and fluxes). Since in each data exchange interval the mass/energy conservation requirement must be fulfilled, an iterative solution must be used. Until a correct solution is found, the same data exchange time step must be used by both models.

The flux quantities that need to be consistent can be calculated in one model and be imposed on the other. For this scheme, two procedures could be used:

- Assume that the state variables in each zone of the multizone model are constant during the envelope model's integration time step and integrate the envelope model while calculating total flux quantities over the adjacent zone interfaces, then consider these flux quantities as sink/source terms in the next calculation step for the multizone model (Fig. 3a).

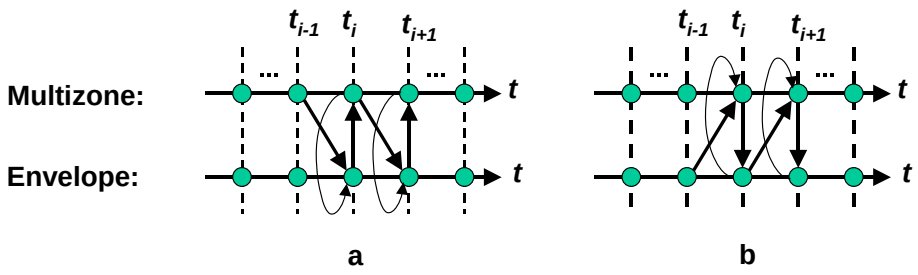

Fig. 3 Coupling schemes in time integration (t_i = current integration time point)

- Integrate the multizone model while calculating total flux quantities into the envelope model (assuming surface conditions to be constant), then integrate the envelope model while imposing the calculated fluxes (as time averaged values) at the boundary (Fig. 3b).

For both methods, the scheme will always conserve mass and energy, regardless of the number of iterations. However, if only one iteration is used, this scheme becomes an explicit coupling scheme for the model on which the boundary/interface fluxes are imposed on. As a consequence, a constraint has to be set on the data exchange time step in order to avoid numerical instability problems. This constraint will depend on how quickly a system reacts to imposed fluxes/sources. The envelope code's (CHAMPS-BES) structure will need to have more storage and redistribution capacity so that it will allow larger time steps if boundary fluxes calculated in the multizone model are imposed on the CHAMPS-BES structure.

For all non-conservative methods the size of the data exchange time step determines the accuracy of the scheme. The advantage of non-conservative methods is the numerical performance and independence of the models, and thus flexibility of coupling different codes together.

Classification based on time stepping control

From code implementation point of view, the coupling methods can be classified based on the approach to the central time step controlling loop:

Option 1: Multizone model controls time stepping ([1] in Fig. 2). The multizone model is at the core of the simulation and envelope components are connected to each zone and deliver on demand interface conditions required for the integration of the multizone model. This approach is in general very good in terms of flexibility and the interface to the envelope code can be quite simple. The envelope code would implement an interface that provides calculated interface conditions (e.g., temperature, RH, pollutant concentration or fluxes) for a given time point based on the history of states in the envelope structure and the zones and current interface variables. Mathematically, this corresponds to adding a non-linear source term to each zone in the multizone model.

However, the major drawback of this approach is the poor performance. Evaluation of the required interface conditions/source terms would demand repetitive integration of the envelope models's time step, which would be very time consuming. Unless some kind of decoupling is used, e.g. by evaluating source terms only at given intervals, this method would result in a major decrease of simulation performance.

Option 2: Envelope model controls time stepping ([2] and [3] in Fig. 2). Two approaches can be used here. The multizone model could be directly integrated into an envelope simulation by simply treating zones as additional elements of a construction with a special treatment during the calculation ([2] in Fig. 2). This would correspond to the direct approach and result in the fastest and most accurate calculation results. However, since the multizone model would need to become part of the envelope code, this would technically no longer be coupling, but rather inclusion and all flexibility for the multizone code development would be lost. The alternative is to call the multizone model during integration/iteration of the envelope model ([3] in Fig. 2). The boundary fluxes calculated for the envelope model can then be treated as non-linear functions of the states in the multizone model. This method would require many re-integration of the current multizone time step. However, since computational costs for evaluating multizone models are typically much lower than evaluating envelope models, this could be a tolerable performance loss.

However, in either case option (2) becomes impractical as soon as two or more envelope structures need to be coupled within a multizone network. It has been attempted to combine all considered envelope structures into a single project and solving all in a combined way (DELPHIN4 HAM simulation tool). Essentially, a single envelope simulation project would then be composed of several envelope structures with each being linked to different zones in the network. This has, however, several disadvantages:

- When adding/removing an envelope structure from the network, the project defining all envelope structures needs to be modified extensively;
- Having all structures defined in one model makes case studies (different wall structures, conditions) difficult and time consuming to set up;
- Simulation time will depend on the slowest structure in the project and require much more operations compared to the approach in which each envelope problem is solved separately.

As a consequence, coupling methods where the envelope code controls the time step is not a recommended solution.

Option 3: Central time stepping control program ([4] in Fig. 2). This method provides most flexibility for coupling different models. Each code would implement a defined interface for the following tasks:

- update necessary boundary/interface variables required for the integration from a shared, central data repository;
- integrate a certain simulation interval;
- update newly calculated interface variables in the data repository for future use by other models.

While this method seems to be the optimal way in terms of flexibility, achieving accuracy would require again some kind of iteration scheme and thus repetitive integration of the multizone and envelope codes. The performance penalties for this approach would also not be tolerable unless explicit coupling can be used. Explicit coupling means that data is exchanged between models only once per integration step, and each time interval is only integrated once. However, the integration of each control time step can be done in each code separately using their respective original iteration scheme. The explicit coupling approach has been used in energy simulation in ESPr, Beausoleil-Morrison (2000).

Selection of method for detailed investigation

Considering the initially presented evaluation criteria, the methods vary mostly with respect to flexibility and simulation performance. All methods requiring repetitive integration, particularly of the envelope models, will have a very poor performance and can be dismissed. The direct coupling method, where the multizone model is directly included into the envelope simulation appears to be superior in terms of accuracy and performance, but would exclude the use of existing multizone codes. Also, the strong dependencies between both codes and models will require much more effort for future extensions.

Considering the remaining options, the conservative method with separate integration and enforced consistence of boundary/interface fluxes seemed a good compromise between accuracy (mass/energy conserving) and performance (no iteration of envelope integration steps needed). Also, the non-conservative method with exchange of interface conditions/states in regular intervals seemed promising, since for small enough interfacing time steps the achieved accuracy would be sufficient. And the flexibility of this method is excellent because the interface can be very small and simple to implement into existing multizone and envelope models. Therefore these variants (**[a], [b] and [c] in Fig. 2)** were further investigated. Each of these variants was implemented and evaluated using a numerical test case, however, only the last method [c] was found to be practical for complex simulation scenarios. For variants [a] and [b] numerical stability required interfacing time steps below 5 minutes (using reasonable discretization of CHAMPS-BES construction), with very poor overall performance. Also, the limiting time step was very dependent on climatic conditions and material properties and difficult to estimate.

IMPLEMENTATION AND RESULTS

In the implementation of variante [c] an interface is defined at each wall surface where temperature, relative humidity and exchange coefficients are stored. Each model uses that data during the given integration interval to calculate boundary fluxes. Additional knowledge about the other coupled models is not required. The interface conditions are calculated by both models and stored in turn in the data structure describing the interface, so that they can be used during the integration of the next model. The principle algorithm is depicted in Figure 4, where a multizone model coupled to two CHAMPS-BES models is integrated.

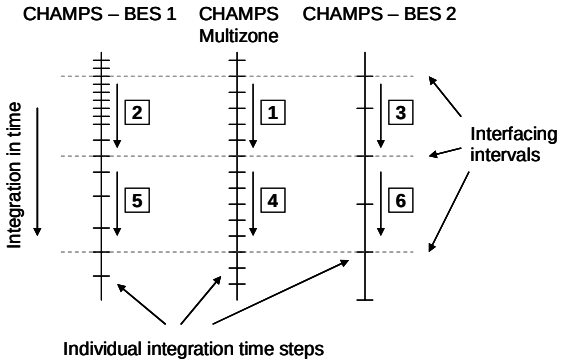

Fig. 4 Integration and interfacing principle

As shown in Figure 4, at first the multizone model is integrated [1], then the zone conditions are stored at the interfaces to CHAMPS-BES models 1 and 2. Next, both CHAMPS-BES models are integrated [2] and [3]. After these models are finished with integration the surface conditions calculated for the CHAMPS-BES models are stored at each interface and the first interfacing interval is complete. Now the multi-zone model can be integrated [4] over the next interfacing interval. Either model can use individual time step sizes during the integration to ensure optimal performance and accuracy in each individual model.

The simulation performance using this method largely depends on the interchange interval lengths (Fig. 5), where simulation times for a one year simulation of a single zone coupled to a one dimensional wall construction is shown, as function of the interchange interval length.

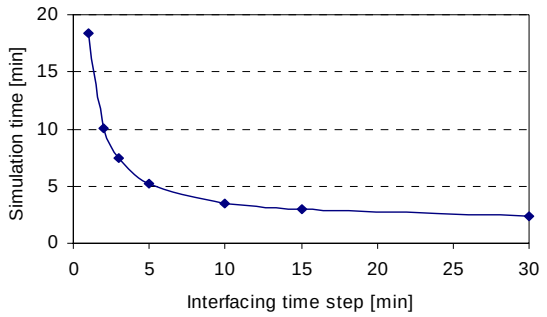

Fig. 5 Simulation performance versus interchange time interval length

Once the exchange time step becomes smaller than the time step used by either model, the performance will greatly reduce. For exchange time steps larger than 30 minutes the simulation times do not change significantly. Long interchange intervals are therefore desirable. However, as mentioned above, accuracy (mass/energy conservation) might still be a problem with this method, particularly for larger interchange intervals. To investigate this, several simulation cases have been run, of which one will be briefly discussed here.

An empty room with a volume of 40 m^3 is modeled, ventilated at 5.4 ach (0.06 m^3/s), with constant inlet relative humidity of 45% and a very simple heating schedule: on April 1, the inlet temperature is turned down from 25 C to 18 C, and at September 15, it is increased again to 25 C. The room has one outside brick wall (surface area 15 m^2), which is exposed to cold and rainy climate in northern Germany (Bremerhaven). The simulation begins on January 1st and continues throughout the year.

Since the relative humidity is of special interest when determining conditions for growing mold and fungi, it is used as one indicator for the quality of the coupled simulation.

While unexpected, the non-conservative method proved to be fairly accurate, even for larger coupling intervals. However, Figure 6 shows clearly the problem with larger interfacing intervals.

While the simulation results for 5 and 30 minute intervals are nearly the same and very accurate compared to the fully coupled solution, the relative humidity calculated with 3 hour intervals shows already small steps. With 12 hour intervals the steps become too large, to be acceptable. Hence, the maximum permissible time step for this simulation was found to be 30 minutes to one hour. This limit is process dependent and will vary depending on the simulation conditions. An approach needs to be developed to adapt the time steps to the specific processes involved, similar to the approach developed by Beausoleil-Morrison (2000) for the coupling between an envelope thermal model and the room CFD model.

Envelope simulations typically require time steps below one hour, yet for performance reasons, the interchange interval lengths should be above 15 minutes. Therefore an exchange time step between 30 minutes and one hour is the recommended compromise between performance and accuracy for this case.

CONCLUSIONS

A systematic analysis has been provided regarding different possible coupling methods, which can be classified based on energy/mass conservation and approach to time stepping control. To allow maximum flexibility in component model development, loose-coupling among component models with central time stepping control appears to

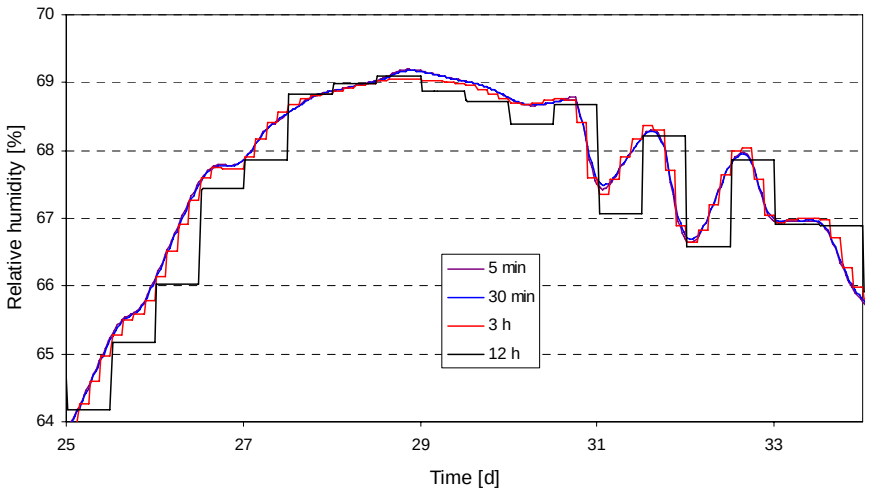

Fig. 6 Stepwise change of zone RH for larger exchange intervals

be most promising. In a case study the most critical parameter for this coupling method and implementation was found to be the coupling/interfacing time step. By selecting proper time steps for exchanging of interface quantities, satisfactory accuracy can be achieved, even if only one round of integration for each exchange time step in the multizone and envelope models (i.e., without iteration) is used.

More realistic cases need to be tested since the suitable coupling time step depends on specific processes being simulated. An intelligent/adaptive time-stepping approach needs to be developed for making the coupling method practical for the wide range of applications.

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