The present challenge for the building industry is to provide buildings that are safe, comfortable, energy efficient and sustainable; creating a healthy and productive environment for users. Computational building performance simulation (CBPS) can play an important role to deal with this challenge, particularly for performance indicators related to the heat, air and moisture (HAM) at the whole-building scale.

In order to improve whole-building HAM accuracy and applicability, this thesis proposes, implements, verifies and validates protocols to integrate building energy simulation (BES) programs and building element heat, air and moisture (BEHAM) simulation programs using external coupling. These protocols, which are based on literature review and theoretical analysis of the governing equations, are implemented in prototype computer programs using numerical simulation and inter-process communication routines. Validation is carried out using analytical solutions, inter-model comparison and experimental results reported in the literature.

Coupled BES-BEHAM simulations showed improvements in the accuracy when compared to stand-alone BES or BEHAM programs. In order to identify cases where coupled BES-BEHAM simulations provide significant improvement in the results, the coupling necessity decision procedure (CNDP) is formulated. Capabilities of coupled BES-BEHAM simulations in combination with the CNDP are demonstrated by case studies, where some capabilities and deficiencies of stand-alone programs are also evaluated.
External coupling of building energy simulation and building element heat, air and moisture simulation

PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Technische Universiteit Eindhoven, op gezag van de rector magnificus, prof.dr.ir. C.J. van Duijn, voor een commissie aangewezen door het College voor Promoties in het openbaar te verdedigen op woensdag 23 februari 2011 om 16.00 uur

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During my first contact with the English language, the meaning of the word “acknowledgement” puzzled me for a while. In English, this word has two distinct meanings that are usually described by different words in Latin languages. The first meaning refers to recognition and acceptance, while the second expresses gratitude. For me, these two meanings are completely unrelated, because the first meaning is a mere observation of fact, as in “He acknowledges that he delivered the package”, while the second meaning is a much more complex concept, expressing the consciousness of having received something that is far above expectations or duties of those you are grateful to. In my native language, the present section would be called “agradecimentos”, i.e. gratitude, which is the actual meaning of this section for me (and for most but not all people). Gratitude is a very special feeling, because it relies only on our expectation of the world. In one hand, if one takes everything for granted, or assumes that other people have the obligation of assisting him/her due to their jobs or their positions in life and society, than there would be nothing to be thankful for. On the other hand, if one understands the miracle of life and human interactions, the acknowledgements would certainly have to be much longer than the contents of the thesis. I tried to keep my acknowledgements to an “acceptable” length, but before I begin I would like to express my true gratitude to all people that have at some moment shared with me the journey that took me to this moment and to this thesis. Albert Camus said once that “Life is a sum of all your choices”, and I would rephrase it a little bit because for me, more than a “sum of choices”, life is also the sum of those with whom we make our choices.

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Summary

External coupling of building energy simulation and building element heat, air and moisture simulation

The present challenge for the building industry is to provide buildings that are safe, comfortable, energy efficient and sustainable; creating a healthy and productive environment for users. Computational building performance simulation (CBPS) can play an important role to deal with this challenge, particularly for performance indicators related to the heat, air and moisture (HAM) at the whole-building scale. These indicators are currently assessed by a large number of programs with considerable uncertainty in their results, such as building energy simulation (BES) programs and building element heat, air and moisture (BEHAM) programs. This thesis poses the hypothesis that the lack of integration between these programs represents an important source of uncertainty in whole-building HAM simulation, which can compromise, in some circumstances, the accuracy of their results. In order to test this hypothesis, this thesis proposes, implements, verifies and validates protocols to integrate BES and BEHAM programs using external coupling. These protocols, which are based on literature review and theoretical analysis of the governing equations, are implemented in prototype computer programs using numerical simulation and inter-process communication routines. The prototypes are verified by a number of techniques developed in this thesis, such as the use of emulators, one-way coupling and self-coupling. Validation is carried out using analytical solutions, inter-model comparison and experimental results reported in the literature. Coupled BES-BEHAM simulations showed improvements in the accuracy when compared to stand-alone BES or BEHAM simulations. In order to identify cases where coupled BES-BEHAM simulations provide significant improvement in the results, the coupling necessity decision procedure (CNDP) is formulated. Capabilities of coupled BES-BEHAM simulations in combination with the CNDP are demonstrated by case studies, where some capabilities and deficiencies of stand-alone programs are also evaluated. This research concludes that coupled BES-BEHAM simulation provides a viable and reliable way to perform whole-building HAM simulation. A number of additional results are also provided in this thesis, such as the solution for several coupling features addressed in the coupling protocols, the verification techniques developed and the use of TCP/IP sockets for the communication between the programs.
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Nomenclature

a – Linear coefficient of heat flux equation (W/K)
b – Independent coefficient of heat flux equation (W)
c – Linear coefficient of moisture flux equation (kg/Pa s)
d – Independent coefficient of moisture flux equation (kg/s)
e – Thickness (cm)
E – Cooling energy demand (MW)
f – Form factor (-)
G – Moisture flux (kg/m²s)
hc – Convective heat transfer coefficient (W/m²K)
hm – Convective mass transfer coefficient (kg/m² Pa s)
hr – Radiant heat transfer coefficient (W/m²K)
m – Measured RH amplitude (%)
p – Predicted RH amplitude using two-way loose coupling (%)
P – Predicted RH amplitude using ESP-r stand-alone (%)
Q – Energy flux (W/m²)
T – Temperature (K)
Ta – Air temperature (K)
Ts – Surface temperature (K)
U – Building element overall heat transfer coefficient (W/m²K)
Δt – Time step (s)
W – ESP-r matrix for each building element
W – Partial vapour pressure (Pa)
R – ESP-r matrix for air node, surface nodes and next-to-surface nodes

Superscripts

\( t \) – Time
\( t+1 \) – Next time step
‘ – Values calculated by ESP-r stand-alone
Subscripts

a – Air
cg – Casual gains
conv – Convection
e – Exterior
out – Exterior
hvac – Heating, ventilation and air conditioning
i – Interior
n – n\textsuperscript{th} surface in a zone
L – Surface position
LW – Longwave
ref – Reference
s – Surface
SW – Shortwave
wdr – Wind-driven rain
Acronyms

ACH – Air changes per hour
AFN – Airflow network
BEHAM – Building element heat, air and moisture
BCVTB – Building controls virtual test bed
BES – Building energy simulation
CBPS – Computational building performance simulation
CFD – Computational fluid dynamics
CNDP – Coupling necessity decision procedure
ECBCS – Energy conservation in buildings and community systems
EMPD – Effective moisture penetration depth
HAM – Heat, air and moisture
HVAC – Heating, ventilation and air conditioning
IAQ – Indoor air quality
IEA – International Energy Agency
IP – Internet protocol
IPC – Inter-process communication
LW – Longwave radiation
PI – Performance indicator
SW – Shortwave radiation
TCP – Transmission control protocol
UDF – User-defined function
Glossary

BEHAM – Building element heat, air and moisture simulation programs are computer programs able to calculate transient conjugate HAM transfer in building elements made of porous materials.

BES – Building energy simulation programs are computer programs able to calculate transient whole-building heat transfer, with no model for moisture transfer or moisture buffering.

Building element – Combination of construction materials, usually arranged in layers, used in buildings for a specific purpose, such as walls, floors, ceilings, floors, windows, vents.

Building envelope – Set of buildings elements aiming to bind the building interior domain, isolating this space from the exterior domain.

Coupled simulation – Simulation performed using two or more CBPS programs.

Exterior domain – Space not bounded by the building envelope.

Interior air node – Representation of the air inside a zone in the building by a single node, assuming that spatial variations in the air temperature and humidity are negligible.

Interior domain – Space bounded by the building envelope and, in some situations, partitioned by additional building elements.

Internal partition – Set of buildings elements aiming to subdivide the building interior domain into rooms.

Model (noun) – A representation of reality, such as physical model (see definition below), a geometrical model (describing the geometrical features of objects), a CBPS program (a combination of different models to represent some features of buildings in the real world).

Model (verb) – Act of creating or using a model.

Modelling resolution – Level of simplification adopted in a model, particularly in comparison to other models. For example, both the Glaser method and BEHAM programs calculate interstitial moisture condensation; however the Glaser method adopts more simplifications than BEHAM programs. Hence, the Glaser method has a lower modelling resolution than BEHAM programs.
Modelling uncertainty – Uncertainty in the results of a model related to the assumptions and simplifications adopted in the model.

Physical model – Model composed by a set of equations which describes the behaviour of some variables involved in a physical phenomenon. The model can be based on first principles (such as the Fourier law) or it can be data-driven (such as the empirical correlations to predict convective heat transfer coefficients).

Physical phenomena – Those related to physics, such as heat, air and moisture transfer, solid and fluid mechanics, and related.

Program – Computer software.

Prototype – In this thesis, prototype refers to a computer program capable of performing calculations, but with no detailed interface and documentation for users.

Stand-alone simulation – Simulation performed using only one CBPS program.

Target value – A value for a given performance indicator that should be met in order to provide a certain required performance. The target value can be a maximum value, a minimum value, or both, defining an interval to be respected. Target values are usually defined in standards, building regulations and etc.

Whole-building simulation – Simulation capable of simultaneously calculate variables in the exterior domain, in the interior domain, in all elements of the building envelope and internal partitions, and in the HVAC domain.
Introduction

1.1 Introduction

The present challenge for the building industry is to provide buildings that are safe, comfortable, energy efficient and sustainable; creating a healthy and productive environment for users (USGBC 2007, ASHRAE 2009). Buildings must be capable of providing this performance not only in the present day, but also in the future, when the building may face different climate scenarios due to global warming (Phillipson and Sanders 2004, Evers et al. 2008). These considerations apply not only for new buildings, but also for renovation projects and for the conservation of historical buildings, where cultural heritage objects should also be preserved (van Schijndel et al. 2008, Steeman 2009, Steeman et al. 2009, van Schijndel et al. 2009). Obviously, this challenge has to be met while respecting social and economical constrains (Jacobs 1961, Montaner 2000, Venturi 2002).

Computational building performance simulation (CBPS) can play an important role to overcome this challenge (Clarke 2001, Hensen and Nakahara 2001, Hensen et al. 2002, Malkawi and Augenbroe 2003). One of the main goals of CBPS is to help practitioners to solve real design problems (Waltz 2000, Turner and Doty 2009), by helping them to take decisions where a large range of options is usually available (Struck et al. 2009). The use of CBPS during the design phase is a highly cost effective alternative to mock-ups and laboratory tests. In the design of whole buildings, mock-ups are usually not feasible. In this case, CBPS remains as the only means to predict the building performance. CBPS is capable of performing this task because it can handle large amounts of data and complex physical models (Clarke 2001). For this reason, it also plays an important role in research, where CBPS is used to improve the overall knowledge about the built environment. When compared to experiments, CBPS requires less cost and execution time (Malkawi and Augenbroe 2003). CBPS also plays an important role in the definition of new standards for building performance (Kokogiannakis et al. 2008), and it is acknowledged as an important teaching resource, providing an environment where young professionals can explore the behaviour of
several physical phenomena in buildings (van Schijndel and Schellen 2009).

There are a large number of CBPS programs available, and new ones are being created to describe specific phenomena in more detail. The development of new and more detailed CBPS programs reduces both uncertainties and costs associated with simulation, consequently allowing its use by more designers and decision makers (Malkawi and Augenbroe 2003). However, new programs rarely address the necessary integration between the different domains involved in the prediction of building performance. The need for an integrated approach of the different scales and physical phenomena relevant for CBPS has been acknowledged by previous studies (Clarke 2001, Hensen et al. 2004). This need is particularly well documented in the case of performance indicators (PIs) related to the whole-building heat, air and moisture (HAM) behaviour (Hagentoft 1996, Hens 1996). The prediction of such indicators involves strong interactions between the three physical domains (HAM) in the three geometrical domains of a building: (1) building exterior, (2) building envelope and interior partitions, (3) building interior (Hens 2005) as represented in Figure 1.1.

**Figure 1.1. Representation of physical and geometrical domains**

Whole-building HAM simulation is important for a detailed analysis of several issues, such as (1) mould on surfaces, (2) decay of wood-based materials, (3) appalling of masonry and concrete caused by freeze-thaw cycles, (4) corrosion of metals, (5) damage from expansion of materials (e.g., bulking of wood floors), and (6) decline in appearance (ASHRAE 2005). This list can be extended to include (7) microbial growth of algae and fungi (Holm et al. 2003, Lengsfeld and Krus 2004), (8) moisture buffering effects (Catalina et al. 2006, Janssen and Roels 2009, Vereecken et al. 2009), (9) indoor air quality (IAQ) and thermal comfort (Toftum et al. 1998, Simonson et al. 2002, Fang et al. 2004) and (10) energy consumption (Abuku et al. 2009d). In spite of the importance of these issues, whole-building HAM simulation still has a high degree of uncertainty, as demonstrated in the next section.
1.2 Uncertainty in whole-building HAM simulation

Current CBPS programs for whole-building HAM simulation have high uncertainty in their results, not only due to input uncertainties but also due to modelling uncertainties. In the present context, modelling uncertainties are those resulting from the assumptions and simplifications adopted in the CBPS programs, rather than the ones resulting from the input used in the simulation.

Relevant examples of modelling uncertainty in whole-building HAM simulation can be found in the results of two comprehensive inter-model comparison exercises. These exercises were carried out in the framework of the Energy Conservation in Buildings and Community Systems (ECBCS) Programme, of the International Energy Agency (IEA). In both cases, a very simple heavyweight building is used in the simulations (BESTEST case 900 building - Figure 1.2) (Judkoff and Neymark 1995, Woloszyn and Rode 2008).

![BESTEST case 900 building](image)

Location: Denver, USA
- $U_{\text{wall}} = 0.5 \text{ W/m}^2\text{.K}$
- $U_{\text{roof}} = 0.3 \text{ W/m}^2\text{.K}$
- $U_{\text{window}} = 3.0 \text{ W/m}^2\text{.K}$
- 0.5 ACH
- Solar heat gain coefficient = 0.78
- Heating set-point = 20 °C
- Cooling set-point = 27 °C

The IEA-ECBCS Annex 43 "Testing and Validation of Building Energy Simulation Tools" was developed to test whole-building energy simulation programs. The main part of this test consists of inter-model comparisons. Figure 1.3 shows the results of annual heating energy demand predicted by different programs, for the BESTEST case 900 building. It is important to note that in these results, only the heat transfer is taken into account, i.e. there is no air or moisture transfer through building elements apart from the fixed air change rate (Judkoff and Neymark 1995). Despite this specific focus and the precise definition of parameters, differences up to 74% can be observed between minimum (1.17 MWh) and maximum (2.04 MWh = 1.17 MWh . 1.74) results obtained from different programs. These results demonstrate the magnitude of modelling uncertainties in whole-building simulation.
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Several programs dealing with energy calculations for the whole building make the assumption that effects of air and moisture transfer through building elements can be neglected. This assumption was investigated by the IEA-ECBCS Annex 41 “Whole Building Heat, Air and Moisture Response”, in which the BESTEST case 900 building, among others buildings, was simulated by CBPS programs that take into account the air and moisture transfer. Results obtained using 13 different programs are shown in Figure 1.4 (dashed line indicates the range of values from Figure 1.3). These results demonstrate that the modelling uncertainty is even higher when air and moisture are taken into account. In the original BESTEST, results were published after a second round of simulations, so that programs with outlier results could correct coding mistakes or assumptions. Results in Figure 1.4 are “blind”, i.e. no adjustment was performed in any program. These results show variations of up to 370%, indicating the relevance of considering air and moisture transfer in energy calculations.

Figure 1.3. Results from several programs for the BESTEST case 900, when only heat transfer is considered (Judkoff and Neymark 1995)

Figure 1.4. Results from several programs for BESTEST case 900, when combined HAM transfer is considered (Woloszyn and Rode 2008)
of moisture transfer and accumulation for at least this particular PI and building. Results for other buildings and PIs show discrepancies of large magnitude as well (Woloszyn and Rode 2008).

It is clearly necessary to improve CBPS programs in order to reduce the uncertainty of whole-building HAM simulation. The next section briefly describes the main types of CBPS programs for whole-building simulation, highlighting their complementary features.

1.3 Programs for whole-building HAM simulation

As discussed earlier in this chapter, CBPS programs generally focus on a specific geometrical domain in combination with one or more physical domains. These programs have strong capabilities, but also some particular deficiencies in terms of boundary conditions, physical models and resolution in space and time. In whole-building HAM simulation, three main types of programs can be identified: building energy simulation (BES) (Crawley et al. 2005), building element HAM simulation (BEHAM) (Hens 1996) and computational fluid dynamics (CFD). The first two are addressed in this research. The role of CFD in whole-building HAM simulation has been addressed by other researchers (Mirsadeghi et al. 2009, Steeman et al. 2009), therefore the present research focus on BES and BEHAM programs, schematically represented in Figure 1.5.

**Figure 1.5.** Representations of BES (left) versus BEHAM (right)

Historically, BES programs, e.g. VABI, ESP-r (Clarke 2001, Strachan et al. 2008) and Energy Plus (Crawley et al. 2001, EnergyPlus 2006), aimed to study the whole-building energy performance and indoor thermal comfort issues. BES programs have
detailed physical models for shortwave (SW) and longwave (LW) radiation, fenestration, bulk air flow through building zones (infiltration and ventilation) and heating, ventilation and air conditioning mechanical systems (HVAC). These programs mainly focus on heat transfer, and as such adopt simplified or no physical models for air and moisture transfer in porous materials (Crawley et al. 2008).

BEHAM programs, e.g. HAMFEM (Janssen et al. 2007), MATCH (Pedersen 1990), WUFI (Künzl 1994), and CHAMPS (Grunewald 1997), provide detailed physical models for the coupled HAM transfer in porous materials. BEHAM simulation is restricted to one element of the building envelope instead of considering, as in BES simulations, the entire building envelope, the interior and the exterior domains (Hens 1996, Hagentoft et al. 2004). On the one hand, moisture transfer modelling is generally a major deficiency of BES programs, but BEHAM programs can calculate moisture transfer in detail (Hagentoft et al. 2004). On the other hand, BEHAM programs have several limitations in the description of interior and exterior boundary conditions, which, in contrast, are comprehensively addressed in BES (Crawley et al. 2008). The combination of the capabilities of BES and BEHAM programs can potentially improve CBPS accuracy, reducing the uncertainty in whole-building HAM simulation.

1.4 Objective

Considering the importance of whole-building HAM simulation and the large uncertainty in the current CBPS programs, it is necessary to reduce the uncertainty in the results of whole-building HAM simulation.

This aim can be pursued using several approaches, such as the development of a new and comprehensive CBPS program or the enhancement of an existing one. However, coupling BES and BEHAM programs seems to be the best option, considering the existing knowledge embedded in these programs and the potential to combine strengths and eliminate some of their deficiencies. The main objective of this research is to develop ways and means to couple BES and BEHAM programs.

Four deliverables are directly related to this objective:

- Coupling protocol

The coupling protocol provides a description of the main aspects involved in the coupled simulations, such as time and space resolution in each program, data exchange frequency, inter-process communication (IPC). The coupling protocol is intended to guide the software development necessary for the coupling implementation.
Prototype software

The prototypes are computer programs capable of performing coupled simulations of BES and BEHAM. They should allow whole-building HAM simulations with a higher level of detail and lower uncertainty, enhancing our knowledge of the building behaviour and performance.

Coupling validation

The coupling validation assesses the validity of the assumptions adopted in the coupling protocol. The validation should demonstrate that coupled simulations provide equally accurate or more accurate predictions than those obtained using stand-alone simulations. In this research, the validation consists of comparisons with analytical solutions, with results from other CBPS programs (inter-model comparison) and with experimental results.

Coupling necessity decision procedure

The coupling necessity decision procedure (CNDP) is a procedure to assist prototype users in determining whether or not a specific building problem demands a coupled BES-BEHAM simulation.

1.5 Hypothesis

This thesis poses the following hypothesis: coupled simulation of BES and BEHAM programs can provide equally accurate or more accurate results in whole-building HAM simulation than stand-alone BES and BEHAM applications.

1.6 Research methodology

Several methods are applied in this research: literature review, analysis of the governing equations, numerical simulation, external coupling, uncertainty and sensitivity analysis.

The literature review investigates key aspects of BES and BEHAM programs, external coupling theory, software development and communication, and finally decision making regarding different modelling resolutions.

The results of the literature review are used in the development of the coupling protocol. In addition, the coupling variables are identified by the analysis of the governing equations, using a deductive approach.

In order to combine BES and BEHAM programs, a technique called external coupling is applied (Hensen et al. 2004, Djunaedy 2005, Trcka (Radoev) et al. 2006,
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Trcka (Radosevic) et al. 2006). External coupling is a method applied to perform a simulation using two or more programs that exchange information in order to model a certain phenomenon. External coupling has several advantages when compared to internal coupling, which is the standard approach to expand a program in order to add a certain missing feature. As shown in Figure 1.6, internal coupling approach involves the choice of an existing physical model or the development of a model (based on first principles or data-driven), extensive code development (the whole added model should be coded), verification of the complete set of new subroutines, validation of the subroutines. Once the new subroutine is developed, it is necessary to integrate it with the existing program and finally to validate the whole new program. In contrast, external coupling significantly reduces the amount of work involved by using previously verified and validated programs. The code development is limited to the communication process and, in some cases, to modifications in the information flow in each program. Finally, external coupling allows the future substitution of one of the programs, if a better alternative or an upgraded version is available.

![Diagram of Internal versus External Coupling](image)

**Figure 1.6. Internal versus external coupling**

The CNDP is based on uncertainty analysis, being the choice for this technique motivated by successful applications of uncertainty analysis to address a similar decision procedure problem (Djunaedy 2005).

1.7 Thesis outline

The thesis is structured as follows:

Chapter 2 describes the capabilities and deficiencies of BES and BEHAM programs. The goal is the identification of complementary features, deficiencies and
potential conflicts between the programs. The result is a schematic overview of the potential role to be played by each program in the coupled simulation.

Chapter 3 addresses the coupling protocols, where all the details necessary for the coupling implementation are described.

Chapter 4 presents the prototype computer programs developed in this research and their verification. Modifications in each code are briefly described, as well as a number of verification exercises used during the prototype development and tests.

Chapter 5 deals with the prototype validation. It includes analytical validation, inter-model comparison and experimental validation.

Chapter 6 presents the CNDP, describing its purpose and utilization.

Chapter 7 shows applications of the prototypes developed in this research, where the CNDP is also applied in the context of two real problems.

Chapter 8 provides a discussion about the outcomes of this thesis. It also summarizes the main conclusions and describes some possibilities for further development in whole-building HAM simulation, particularly concerning the coupling of BES and BEHAM.
1. Introduction
2

Capabilities and deficiencies of BES and BEHAM programs

2.1 Introduction

Although dealing essentially with the same phenomena in buildings, research groups in charge of the development of BES and BEHAM programs are traditionally part of different research communities. This separation is clear when one compares the International Building Performance Simulation Association (IBPSA) and the International Building Physics Association (IBPA). Roughly, it could be said that these two associations host many of the members of BES and BEHAM communities, respectively. They have their own conferences and their own international journals. This separation was beneficial during the early stages in the development of BES and BEHAM programs, mainly because these programs have different spatial and temporal scales. However, recent projects have reduced the distance between these two communities due to the growing need to take into account the interactions between these scales. These projects are described in Sections 2.2 and 2.3, respectively for BES and BEHAM programs, while Section 2.4 summarizes previous studies on the integration of BES and BEHAM. In spite of these studies, there is still a large gap to be overcome (Woloszyn and Rode 2008). This gap is demonstrated by the comparison of features included in one BES program and one BEHAM program, both state of the art in their field. Section 2.5 describes the selection of these two programs, and Section 2.6 contrasts the main capabilities that are available in each one of the selected program. The goal is to identify complementary features and potential conflicts between these programs in order to define the coupling protocol in Chapter 3. The result is a schematic overview of the potential role to be played by each program in the coupled simulation.

2.2 Recent developments and trends in BES programs

Two large projects were conducted by the BES community in the recent past to compare different BES programs: the BESTEST (Judkoff and Neymark 1995) and a
The BESTEST project created a benchmark for BES programs, based on the comparison of results of state of the art BES programs (Judkoff and Neymark 1995). It uses cases of increasing complexity to isolate and diagnose problems in BES codes. The BESTEST was later adopted in a standard (ASHRAE 2007), but in spite of its importance it does not take into account any air and moisture transfer through building elements. In BESTEST, the focus is on the results, not on the individual capabilities of each program.

Another recent study compared BES programs focusing on their capabilities and physical models (Crawley et al. 2005, Crawley et al. 2008). From the 16 programs addressed in this study, 8 declared themselves to be able to perform “moisture transfer” calculations. However, the study does not give any further attention to the details of the moisture transfer calculation, indicating that moisture transfer is not a primary concern in this study (Crawley et al. 2005, Crawley et al. 2008). Indeed, the moisture transfer calculation in BES programs is performed using quite different and often simplified approaches. While most of the programs have coupled heat and moisture transfer models with no liquid transfer, at least one program considers as “moisture transfer” the use of the Glaser method to assess the risk of interstitial condensation. This is an indication of the simplicity of moisture transfer models in BES when compared to the state of the art BEHAM programs.

Whole-building moisture simulation presents some additional challenges in BES programs. The simulation of HVAC systems with capabilities to control moisture levels in the room is not a default feature in many BES calculations. In warm humid countries, the latent load in cooling coils is particularly important, but basic controls in BES focused only on heat do not take into account this aspect. Moisture source profiles in time are usually not available in BES, but the importance of these loads has been acknowledged by previous studies (Kalamees et al. 2005, Saito 2005). The performance of some HVAC systems can be greatly influenced by moisture related phenomena (e.g. moisture buffering) that are not usually taken into account in BES (Catalina et al. 2006). On the other hand, moisture in indoor environments strongly depends on the ventilation rate (Kalagasidis 2006, Berthin et al. 2007), which can be calculated by BES with good accuracy. Deficiencies in the moisture calculation in BES programs can be attributed to the development process of these programs, which must address a very large number of topics in all physical and geometrical domains, as shown in Figure 1.1.
Some of the current research that may in the future be available in BES programs includes a broad range of topics, such as:

- Uncertainty in bulk air flow calculation and unsteady effects (Cóstola and Etheridge 2008, Cóstola et al. 2009).
- Integration with CFD in the exterior domain (Blocken et al. 2009a, Defraeye et al. 2010).
- Integration with CFD in the exterior and interior domains (van Hooff and Blocken 2010).
- Modelling of innovative HVAC systems (Henninger et al. 2004, Trcka and Hensen 2010).
- Advanced fenestration models (Lomanowski and Wright 2009).
- Optimization (Hopfe 2009).

The amount of research in the BES community demonstrates the existence of space for improvement in BES programs. The next section discusses development of BEHAM programs towards whole-building HAM simulation.

2.3 Recent developments and trends in BEHAM programs

Over the last decades the BEHAM community has developed several common projects investigating whole-building HAM simulation.

The IEA-ECBCS Annex 24 "Heat, air and moisture transfer in insulated envelope parts (HAMTIE)" studied the state of the art in BEHAM programs based on the identification and comparison of 37 BEHAM programs (Hens 1996). The comparison showed significant differences between programs and highlighted areas where BEHAM performance could be improved. For example, although several of the programs were able to handle 1D or 2D problems, none were capable at that time of solving problems in 3D. Heat transfer calculation capabilities were based on similar assumptions in most programs. The same applies for moisture transfer, where most of the programs were able to perform transient vapour and liquid transfer, but only two of them were capable of modelling hysteresis. Only a small number of programs were able to take into account air transfer.
2. Capabilities and deficiencies of BES and BEHAM programs

The HAMTIE project also quantified the importance of HAM effects on building energy demand and building element durability (Hagentoft 1996). The study concludes that BEHAM results are significantly more accurate than simplified calculations methods, based only on transient heat transfer or on steady state heat and moisture calculations (Hagentoft 1996). This project was an important step towards performance-based design and analysis of moisture related problems in buildings.

In the European project HAMSTAD (Hagentoft et al. 2004), a set of BEHAM programs were compared using more comprehensive exercises. The project intended to define benchmarks for the validation of BEHAM programs. Compared to HAMTIE, the number of programs involved was smaller: seven programs were evaluated. The exercises comprised 1D problems, with no water to ice phase change in the construction. No hysteresis was considered, and wind-driven rain was treated in a simplified way. Results showed good agreement between most of the programs.

BEHAM programs described in HAMTIE and HAMSTAD projects did not include research in HAM transfer carried out in the last years. Partially, it is because these projects are relatively old. Partially, it is because there is a large delay between research and implementation in CBPS programs in general (Malkawi and Augenbroe 2003). This delay, which is also present in BES, makes the use of external coupling very attractive, because maintaining and upgrading two separate codes with a smaller scope is much simpler than one large and comprehensive code. This means that BEHAM and BES communities can work separately developing their codes and keeping them as up-to-date as possible.

Some of the current research that may in the future be available in BEHAM programs include a broad range of topics, such as:

- Anisotropic materials (Zillig et al. 2007).
- Material interface effects (Janssen et al. 2007).
- Material properties for indoor finishing materials and furniture (Svennberg 2004).
- Coupling of mechanical and transport models for damage analysis (Roels et al. 2006, Carmeliet et al. 2008).

- Improved simulation of air transfer through the envelope (Umeno et al. 2006, Li et al. 2007).

The amount of research in the BEHAM community demonstrates the existence of space for improvement in BEHAM programs. Material properties, for example, are a major concern in BEHAM programs. There are numerous experimental techniques in use to obtain material properties, and more techniques are under development in order to reduce the uncertainty in measurements (Roels et al. 2004, Scheffler 2008). In most cases, these techniques do not result in transport properties. Instead, HAM experiments provide intermediary results that are used to calculate transport and storage parameters, the so-called material modelling. Material modelling can be done in several ways, leading to a variety of parameters and transport equations that essentially describe the same phenomena (Scheffler 2008). In this sense, efforts to compile extensive material databases (e.g. Kumaran 2006), will probably be repeated in the future using more accurate techniques. Moreover, new material modelling techniques might lead to new HAM transfer models, and consequently new BEHAM programs (Kumaran and Normandin 2004, Scheffler 2008, Steeman et al. 2009).

Uncertainties in BEHAM modelling are also related to difficulties in validating BEHAM programs. It is a complex and time-consuming task (Maref et al. 2003), performed in most cases under controlled conditions (e.g. Maref et al. 2003, Fazio et al. 2006). However, validation under controlled conditions can mask deficiencies on BEHAM program, such as deficiencies related to the use of atmospheric boundary conditions regarding a number of processes taking place on the building facade, such as direct, diffuse and reflected income of SW radiation, LW radiation from the sky, from the surrounding buildings and from the ground surface, convective heat and mass transfer, wind-driven rain and run-off. In HAMSTAD projects, for example, there was no common exercise addressing atmospheric boundary conditions. This kind of exercise could expose limitations of some BEHAM programs in this aspect when compared to BES programs. Boundary conditions are usually case dependent (building and surroundings geometry, flow regime, etc); therefore their calculation requires knowledge not only on the building element scale, but also on the whole-building scale. The next section reviews previous research dealing with the integration of BES and BEHAM programs.
2.4 Previous studies on the integration of BES and BEHAM

Due to the strong interaction between the phenomena covered by BES and BEHAM programs, some studies were conducted in the past in order to include features of one program into the other. These previous studies are discussed in this section.

Several BES programs, which initially only included heat transfer calculation, were expanded to perform coupled heat and moisture calculation, e.g. Energy Plus (EnergyPlus 2009) and ESP-r (Nakhi 1995). As described in Section 2.2, most of these programs adopt large simplifications in HAM modelling. In several cases, the HAM implementation is limited to moisture buffering calculation, which can be performed using isothermal vapour transfer models (Steeman et al. 2009, Steeman et al. 2010). Liquid transfer, for example, is usually not taken into account. An exception is Energy Plus, which has been recently upgraded with a heat and moisture transfer model, which works with the original BES program using internal coupling (EnergyPlus 2006, EnergyPlus 2009). This model is not the default Energy Plus engine, and it is described as “Advanced/Research usage” (EnergyPlus 2009). It performs 1D calculations including liquid transfer in the building envelope, using the finite element method. In terms of heat and moisture calculation, the new Energy Plus engine represents a significant improvement compared to previous BES programs. However, Energy Plus has some limitations when compared to state of the art BEHAM programs, such as the restriction to 1D calculations, the absence of adaptative time steps, hysteresis modelling, a very limited material database and no air transfer. Moreover, validation of this code could not be found in the Energy Plus documentation and references (EnergyPlus 2009).

Some BEHAM programs were extended to perform whole-building simulation, by allowing simultaneous simulations of several building elements and by including the energy balance of the interior air node. For example, the BES programs WUFI-Plus and CHAMPS Multizone were based on the BEHAM program WUFI and CHAMPS (Holm et al. 2004, Nicolai et al. 2007). In both cases, internal coupling was adopted. This approach is used by most program developers, not only in BES but in CBPS in general. It has several advantages, such as keeping a uniform code structure. The drawback is the large effort necessary to expand the program capabilities, as described in Section 1.6. WUFI-Plus and CHAMPS Multizone do not include some standard features present in other BES programs described in Crawley (2005), such as a comprehensive HVAC modelling, solar processor for exterior obstructions and for solar distribution in the zone level, detailed view factor calculator.
Most research in the combination of BES or BEHAM has concentrated so far on one-way coupling, i.e. boundary conditions calculated using BES are used as input in BEHAM simulations (Koronthalyova et al. 2004, Moon 2005). This approach can produce useful boundary conditions for BEHAM when the indoor conditions are dominated by the HVAC system, as will be demonstrated in Chapter 5. However, it is less advantageous for the calculation of PIs on the whole-building level, such as energy demand and peak power demand.

The use of CFD for HAM simulation in buildings has increased in the recent past, and it represents an important alternative for the prediction of HAM related PIs. However, whole-building simulation is still not feasible using this approach due to, among others, the large computational resources required by CFD (Hedegaard et al. 2004, Steeman et al. 2009).

Another important approach to whole-building HAM simulation is the use of Matlab based CBPS programs (Hagentoft and Kalagasidis 2003, Tariku et al. 2006, de Wit 2008). They provide a very straightforward platform for CBPS development (especially when compared to Fortran or C), due to a large number of functions available and the capability of running parts of the code directly in the software development environment. However, quality assurance issues should be carefully evaluated because it is usually necessary to modify the source code in order to setup simulations.

Most of the CBPS programs described in this section were used in the IEA-ECBCS Annex 41, a recent project which studied HAM topics at the whole-building scale (Hens 2005). Initially, the BESTEST was applied by all the participants in the "Common exercise 0, BESTEST digest". In this exercise, only 2 out of 13 programs provide all results within the range specified by BESTEST. It was concluded that "deviation of results within a reasonable range gives further confidence in the energy models" (Woloszyn and Rode 2008), which might be seen as a too optimistic conclusion. Whole-building HAM simulations were performed in the "Common Exercise 1 - BESTEST REVISED". The first draft of the exercise was very ambitious in the range of phenomena to be addressed. However, discrepancies in the first round of results made clear that the "exercise should get redesigned to be significantly simpler" (Rode and Peuhkuri 2005). In addition, some features, such as wind-driven rain, were not considered in order to allow the participation of simulation programs that could not handle liquid transfer. The results of Annex 41 provide a valuable overview of the state of the art in
whole-building HAM simulation. They also indicate that whole-building HAM simulation suffers from large uncertainties.

### 2.5 Selection of BES and BEHAM programs

In order to reduce the uncertainty of whole-building HAM simulation, this research defines, implements and validates protocols to couple existing BEHAM and BES programs. Initially, a selection of suitable candidates (BEHAM and BES programs) for the coupling was performed. Three criteria were adopted: firstly, the programs should represent the state of the art in their field; secondly, a previous and extensive validation of each program was mandatory; thirdly, the source code of each program should be available. Considering these requirements, the programs chosen for this research were the BES program ESP-r (Clarke 2001) and the BEHAM program HAMFEM (Janssen et al. 2007).

ESP-r is a leading scientific BES program (Clarke 2001). It is open source free software written in Fortran 77/90 and distributed under the GNU General Public License. ESP-r has an active development community, and the code maintenance is done using state of the art programs to manage the contributions of different developers, to test the code quality regarding syntax and to test the code results in benchmark cases. ESP-r is a code with more than three decades of continuous development; it has a simple graphic interface and extensive quality assurance procedures. Another positive point in ESP-r structure is its modularity, so the code related to air flow network or HVAC systems is completely separate from the core module, responsible for the building heat balance.

HAMFEM is a 3D BEHAM program developed at the K.U. Leuven using the finite element method (Janssen et al. 2007). As many academic codes, the program is written in Fortran 90, has no graphical interface and no quality control by the program over the correctness of input data provided by users. One important feature is the high level of hardcoded information in the program, e.g. material properties and the boundary conditions are implemented directly in the code for each case to be simulated. This feature represents a serious limitation in terms of quality assurance because the code should be verified and validated every time it is changed, i.e. every new simulation would demand verification and validation of the whole code. Nonetheless, it does facilitate the coupling with other programs, because the coding process for boundary condition implementation is better documented than in other CBPS source codes.
Before using the codes, benchmark exercises such as BESTEST and HAMSTAD were partially reproduced in order to guarantee that the codes comply with the results, and also to guarantee that the author of this thesis was able to reproduce benchmark results.

2.6 Capabilities and deficiencies of ESP-r and HAMFEM

In order to establish the role of ESP-r and HAMFEM in the coupled simulation, an investigation was performed regarding their capabilities and deficiencies. This investigation was based on the documentation and codes of both programs. Table 2.1 lists some aspects that are extensively implemented and validated in ESP-r or HAMFEM programs. The list is restricted to the aspects that are addressed in only one of the programs in order to clarify their complementary characteristics. For example, both ESP-r and HAMFEM are able to calculate the incoming shortwave (SW) radiation in a given surface, and this capability is not included in Table 2.1. However, only ESP-r can take into account the obstruction of SW radiation by neighbours, therefore this capability is included in Table 2.1.

The modelling of relevant physical phenomena taking place in the exterior domain is more comprehensive in ESP-r than in HAMFEM for several, but not all, aspects. In particular, the highly developed solar processor in ESP-r is capable of modelling the effect of various obstructions for various elements of the building envelope, independent of their orientation. Therefore, ESP-r is the best option to model all aspects of the exterior domain, except wind-driven rain. In addition to the database of catch ratios provided by HAMFEM, the lack of support for rainfall intensity in native ESP-r weather files (Crawley et al. 1999) presents a major constraint for the use of ESP-r to calculate wind-driven rain load.

The modelling of relevant physical phenomena taking place in the building envelope and interior partitions modelling is much more comprehensive in HAMFEM than in ESP-r, providing detailed coupled calculation of all physical domains. However, two capabilities of ESP-r are not available in HAMFEM, and in some cases they might be particularly important for the simulation results and efficiency. The first one deals with the simultaneous calculation of all building elements in a zone, using a single matrix. This aspect improves the efficiency of ESP-r calculation of heat transfer, allowing large time steps (up to one hour). The second aspect in the building envelope provided only by ESP-r is crucial for the simulation of a number of realistic building cases: the possibility of heat injection in nodes inside building elements. This feature is essential.
for the simulation of any building element in which pipes or electrical resistances deliver energy inside floors, walls or ceilings. Based on Table 2.1, it can be concluded that HAMFEM is the best option to model the building envelope and internal partitions whenever there is no heat injection inside building elements. It is however possible that a future version of HAMFEM might have facilities for heat injection in nodes inside building elements.

### Table 2.1. Features extensively addressed in ESP-r or in HAMFEM

<table>
<thead>
<tr>
<th>Geometrical domain</th>
<th>Physical domain</th>
<th>Phenomenon / modelling techniques</th>
<th>ESP-r</th>
<th>HAMFEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exterior</td>
<td>Heat</td>
<td>SW radiation:</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Obstruction by neighbours (direct and diffuse)</td>
<td></td>
<td>X</td>
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<tr>
<td></td>
<td></td>
<td>Ground reflected component</td>
<td></td>
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<td></td>
<td></td>
<td>Anisotropic sky model for diffuse radiation</td>
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<td></td>
<td></td>
<td>LW radiation:</td>
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<td></td>
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<tr>
<td></td>
<td></td>
<td>Surrounding building effect</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Calculated ground surface temperature</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>Convection: Several empirical models</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>Building Envelope</td>
<td>Air</td>
<td>Pressure coefficient: Database and empirical models</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>and Interior</td>
<td>Moisture</td>
<td>Wind-driven rain: Catch ratio database</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>Partitions</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>Simultaneous calculation of heat transfer through all building elements in a zone</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td></td>
<td>Heat</td>
<td>Heat injection/extraction in one wall node as function of the state of another node in the zone</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Coupled calculation with other physical domains (air and moisture) in 3D</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td></td>
<td>Air</td>
<td>Air transfer through homogeneous porous media</td>
<td></td>
<td>X*</td>
</tr>
<tr>
<td></td>
<td>Moisture</td>
<td>Liquid transfer</td>
<td></td>
<td>X</td>
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<tr>
<td></td>
<td></td>
<td>Condensation</td>
<td></td>
<td>X</td>
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<tr>
<td></td>
<td></td>
<td>Hysteresis</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>Interior</td>
<td>Heat</td>
<td>LW radiation:</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Raytracing view factors</td>
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<td></td>
<td></td>
<td>Calculated temperature for surrounding surfaces</td>
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<tr>
<td></td>
<td></td>
<td>SW radiation: Sun penetration through windows</td>
<td></td>
<td>X</td>
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<tr>
<td></td>
<td></td>
<td>Convection: Several empirical models</td>
<td></td>
<td>X</td>
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<tr>
<td></td>
<td></td>
<td>Schedules for internal gains</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td></td>
<td>Air</td>
<td>HVAC system</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Air Flow Network (AFN)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

X* - Limited capabilities compared to some BEHAM programs

The interior domain modelling in ESP-r is much more comprehensive than in HAMFEM. ESP-r provides several facilities for whole-building simulation, such as HVAC systems, infiltration and ventilation calculation using airflow network (AFN). It also calculates SW and LW radiation in detail. Based on Table 2.1, it can be concluded that, compared to HAMFEM, ESP-r is the best option to model all aspects of the interior domain.
2.7 Conclusions

The literature review presented in this chapter allows the following conclusions to be made:

- In spite of the efforts in the development of BES and BEHAM programs, there is no program that combines the capabilities of state of the art programs in both fields, allowing detailed whole-building HAM simulation.

- ESP-r and HAMFEM have the pre-requisites for coupled BES and BEHAM simulation (i.e. state of the art models, extensive validation, source code available).

- ESP-r has more comprehensive capabilities to model the exterior domain, however HAMFEM has some features that are not available in ESP-r, such as the wind-driven rain boundary condition.

- HAMFEM has more comprehensive capabilities to model the domain of the building envelope and internal partitions; however ESP-r has some features that are not present in HAMFEM, such as the injection of heat in intra-wall nodes.

- ESP-r and HAMFEM can model unique and distinct aspects in both the exterior and the building envelope domain, and they should, if possible, be combined to model these geometrical domains.

- Interior domain modelling in ESP-r is more comprehensive than HAMFEM in all aspects, and ESP-r should be used to model this geometrical domain.
2. Capabilities and deficiencies of BES and BEHAM programs
Coupling protocols

3.1 Introduction

As described in Chapter 1, external coupling is a method applied to perform a simulation using two or more programs that exchange information in order to model a certain phenomenon. A number of features should be considered before performing such a coupled simulation, such as time and space resolution in each program and data exchange frequency. These features are addressed in the coupling protocols. The concept of coupling protocol is introduced in this thesis to formalize a set of features and solutions relevant for the coupled simulation, consequently serving as a guide for the coupling implementation. In this sense, the coupling protocol provides a high level description of solutions, which should not be program specific, but rather generally applicable for most of BES and BEHAM programs. The intention of a protocol is to provide the means to separately modify and test each of the programs concerning the coding necessary to perform coupled simulations. Once both programs are modified and tested, a coupled simulation can be performed using both programs simultaneously.

Coupling features consist of different aspects involved in the coupling, e.g. geometrical, physical, mathematical and computational. In this chapter, the following coupling features are addressed:

- Coupling interface node.
- Domain overlap.
- Geometrical features.
- Coupling variables.
- Coupling mode.
- Coupling strategy.
- Coupling frequency.
- Inter-process communication (IPC).
A more comprehensive and general discussion about coupling features can be found in Trcka et al. (2009). The next sections provide a discussion about coupling features focused on BES-BEHAM coupled simulation. At the end of this chapter, three coupling protocols (A, B and C) are established (see Section 3.10) and Chapter 4 describes the implementation of these protocols in prototype computer programs.

### 3.2 Coupling interface node

The coupling interface node(s) describe(s) the point(s) in space in which the two programs exchange information. In BES-BEHAM coupling, at least four solutions are identified in this thesis:

- Interior air node.
- Interior surface node.
- Interior and exterior surface node.
- All nodes in the building element.

The first option is the simplest alternative to exchange information between BES and BEHAM, because it does not require any modification in the codes. This option is usually applied when BES provides data to BEHAM about the states (temperature, humidity and pressure) of the interior air node. This option poses severe limitations concerning the coupling variables that can be adopted. For example, SW and LW radiation in the interior domain cannot be included in the coupling because they are not functions of the air temperature. Due to the widespread use of indoor air node as coupling interface node, it was considered important to adopt it in one of the coupling protocols developed in this thesis (coupling protocol A). The main intention was to clarify the shortcomings related to this option.

The second option is an enhanced version of the first one, but in this case BES models all phenomena related to the interaction between the building element surface node and the surrounding environment (including the SW and LW radiation). This option provides a stronger interaction between BES and BEHAM than the previous option, but also requires modifications in both source codes.

The third option is, in turn, an enhanced version of the second option. In this case, both interior and exterior geometrical domains are completely calculated by BES. This option preserves the main capabilities of BES and BEHAM described in Table 2.1. For this reason, this option is adopted in two of the three prototypes developed in this thesis (coupling protocols B and C).
The fourth option describes the exchange of information between all nodes of the building element. This option could potentially be capable of preserving all capabilities of BES and BEHAM; however this option has many drawbacks. Among others, this option would require in-depth modifications in the codes, it would involve the exchange of large amount of information and stability problems could be expected. Hence, benefits of external coupling are reduced, and for this reason this option is not included in this thesis.

The choice for a certain interface node is closely related to the domains covered in each program to be coupled. The domains addressed in BES and BEHAM are discussed in the next section.

### 3.3 Domain overlap

In general, coupled simulations are used when each program models one specific domain. However, in some cases both programs model the same geometrical or physical domain, i.e. there is a domain overlap that should be addressed in the coupled simulation. This thesis identifies that it is the case in BES-BEHAM coupling, because both programs are dedicated to the calculation of the temperature distribution inside the wall, using, however, different sets of equations. While in BES only the Fourier equation is solved in 1D, BEHAM programs solve a more comprehensive set of coupled equations of HAM transfer in 1D, 2D or 3D. Here, two possible approaches to solve the domain overlap problem are introduced: suppression of the overlapped domain in the BES program, or the synchronization of both programs in the overlapped domain.

Figure 3.1 schematically represents the suppression of the overlapped domain in BES. It is simple in nature, but complex to implement because it involves some modifications in the problem description in the BES program. In spite of this complexity, suppression is advantageous because then the programs only need to exchange information for a few interface nodes.

Figure 3.2 schematically represents the synchronization of domains. Here, both programs calculate the temperature distribution inside the wall and exchange data for all these nodes. In this case, the heat transfer equations in the BES program should be modified to include moisture related terms, such as heat storage, changes in the thermal conductivity and sink/source terms for latent heat. Although possible, synchronization presents no net benefits because of the following considerations: 1) it requires deep modifications in the problem description in the program; 2) the number of interface nodes is much higher when compared with the suppression approach, and
3) stability and convergence problems can be expected due to the strong interaction between the BES and BEHAM programs.

**Figure 3.1. Suppression of the overlapped domain**

**Figure 3.2. Synchronization of the overlapped domains**

Considering the advantages and disadvantages of suppression of the overlapped domain and of synchronization of the overlapped domain, it is clear that the suppression of the overlapped domain in the BES program is the best alternative to solve the domain overlap problem. Therefore, in this thesis, the suppression of the overlapped domain in the BES program is adopted in coupling protocol C. The implications of this approach for the modifications in the BES code are discussed in Chapter 4. For the coupling protocols A and B, the domain overlap is not an issue as it will be discussed in Section 3.6. The solution of domain overlap problems is directly related to the level of detail in the geometrical features used in BES and BEHAM, which are described in the following section.
3.4 Geometrical features and 1D versus 2D-3D simulation

Most BES programs calculate heat transfer through building elements in only 1D, while many BEHAM programs can also provide 2D or 3D calculations. The difference in dimensions in BES and BEHAM programs does not represent a problem, because it is possible to run a 1D simulation in most of the BEHAM programs, so the problem description is done at the same level in both programs. In this thesis, all simulations are carried out in 1D. However, two issues should be highlighted concerning this.

Firstly, the adequacy of air transfer modelling in 1D is very limited for lightweight constructions. In these constructions, air transfer might occur through joints, and there is buoyancy driven flow inside the wall, therefore 2D or 3D are necessary. Li et al. (2007) provide a good example of the importance of 2D effects in air transfer in building elements. Secondly, BES programs usually treat the building elements as a single entity, i.e. the whole wall is considered as a single element, with uniform state and boundary conditions over the whole surface. This approach compromises the analysis of local problems such as mould growth and condensation in spots near edges and corners. The discretization of the building elements in several co-planar 1D elements, the so-called surface discretization as presented in Figure 3.3, does not necessarily improve the accuracy of the predictions. There might be no improvement due to the use of empirical models to estimate surface averaged convective heat transfer coefficients by BES programs. These models often require the surface length as input. The length of the surface is reduced by the discretization, therefore surface-discretized BES tends to overestimate the transfer coefficient. Coupling with CFD can overcome this limitation, which could make surface discretization a useful strategy when coupling BES, BEHAM and CFD programs.

3.5 Coupling variables

The correct definition of variables to be exchanged between different programs is a key task in coupled simulations. This task is carried out based on the analysis of the governing equations used in both programs. In some cases, variables can be easily
mapped. However, there are cases where the same variable is defined in different ways in each program (Djunaedy 2005). In BEHAM programs, there is no consensus about the driving potential for the moisture flux, so it is hard to define coupling variables that are not program specific (Hens 1996). However, driving potentials used in different BEHAM programs can be easily converted.

As described in Section 3.2, the building element surfaces, i.e. the boundary condition nodes in BEHAM, are defined as the interfaces nodes between BES and BEHAM programs. In the BEHAM program, the boundary condition can usually be defined in two forms:

- State (Dirichlet boundary condition).
- Flux (Neumann boundary condition).

While both forms are possible, the use of the Neumann boundary condition for the BEHAM program is particularly suitable for coupling with BES programs. The Neumann boundary condition allows the BEHAM program to calculate the states at the surface node, taking into account phase changes at this node that clearly influence its states. Subsequently, the BES program can use the states calculated by the BEHAM program as the boundary condition, and perform the calculation to obtain the fluxes of each quantity at the surface. In most cases, air flux through porous materials in building elements is negligible compared to the air mass balance in the zone level. Therefore BEHAM does not send any information to BES regarding this physical domain and for this domain one-way coupling is performed. Figure 3.4 summarizes the coupling variables for BES-BEHAM coupling.

<table>
<thead>
<tr>
<th>BES</th>
<th>BEHAM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat</td>
<td></td>
</tr>
<tr>
<td>Heat flux (W/m²) as function of the surface temperature</td>
<td>Surface Temperature (K)</td>
</tr>
<tr>
<td>Moisture</td>
<td></td>
</tr>
<tr>
<td>Moisture flux (kg/m²s) as function of the partial vapour pressure</td>
<td>Partial vapour pressure (Pa)</td>
</tr>
<tr>
<td>Air</td>
<td></td>
</tr>
<tr>
<td>Air pressure (Pa)</td>
<td></td>
</tr>
</tbody>
</table>

**Figure 3.4. Coupling variables**

The Neumann boundary condition could be imposed in two different ways in BEHAM:
- Integrated flux, which is pre-calculated by BES based on the surface state available from the previous data sent by BEHAM.

- Flux equation, where the integrated flux can be calculated by BEHAM using up-to-date data of the surface node state.

The integrated flux consists of the sum of all fluxes at the surface, as exemplified in Figure 3.5. Only this integrated flux is sent by BES to BEHAM and then used as the boundary condition.

![Figure 3.5. Scheme representing the integrated flux](image)

For the heat flux, the integrated value to be delivered to the BEHAM program is defined by Eq. (3.1):

\[
Q_t^i = Q_{SW-i}^i + Q_{cg}^i + Q_{hvac}^i + Q_{conv}^i + Q_{LW}^i
\]

(3.1)

where \( Q_{SW-i}^i \), \( Q_{cg}^i \), and \( Q_{hvac}^i \) are, respectively, the gains due to SW radiation, casual gains due to occupancy, equipments and lighting, and the radiant fraction of the HVAC system. The convective component of the HVAC system is taken into account by the air temperature in the zone. The terms \( Q_{SW-i}^i \) and \( Q_{cg}^i \) are independent of the surface temperature (\( T_s \)), while \( Q_{hvac}^i \) depends on \( T_s \) but this dependence is not taken into account in this thesis. The terms \( Q_{conv}^i \) and \( Q_{LW}^i \) are the gains due to convection and LW radiation, respectively, which are both dependent on \( T_s \). Considering that \( T_s \) is calculated by BEHAM, BES can only calculate the integrated flux by using \( T_s \) sent by BEHAM in the previous data exchange between the programs.

Obtaining the integrated flux is straightforward, because many BES programs provide post-processing facilities to calculate the heat flux at a given node. However, the use of integrated values in BEHAM programs has two drawbacks. The first is the delay due to the use of flux values calculated by BES based on the state at the previous data exchange with BEHAM. The second, and more important, is the adoption of the “Newton-Raphson” scheme by some BEHAM programs, e.g. HAMFEM. This scheme improves the convergence of the highly non-linear coupled equations of HAM transfer in
the building element, but it is based on the use of derivatives to solve the system of equations. It means that BEHAM programs using the "Newton-Raphson" scheme do not accept integrated flux as the Neumann boundary condition, necessarily requiring a function where the derivative of $Q_t^i$ in $T_s$ is known. In such cases, this thesis identifies the need to describe boundary conditions in the flux equation form.

The flux equation describes the total flux as a function of the surface state, so additional parameters should be extracted from BES, as represented for the case of the heat flux in Figure 3.6. Some additional values that should be extracted from BES are the convective heat transfer coefficient ($h_c$), air temperature ($T_{air}$), all surface temperatures ($T_{s-n}$) and the view factors ($f_n$).

![Figure 3.6](image)

**Figure 3.6 . Scheme representing the some parameter of the flux equation**

The heat flux equation (Eq. (3.2)) is described below:

$$Q_t = Q_{SW}^i + Q_{cg}^i + Q_{hvac}^i + Q_{conv}(T_{s}^i) + Q_{LW}(T_{s}^i)$$  \hspace{1cm} (3.2)

where $T_{s}^i$ is unknown and will be calculated by the BEHAM program.

From the discussion above, it is clear that obtaining the flux equation requires more information than is required to calculate the integrated flux. Here, modifications in the source code are probably necessary. The final equation, however, is very simple, because all terms in Eq. (3.2) are linear or can be cast into the linearized format, so independent and dependent terms can be grouped, resulting in Eq. (3.3):

$$Q_t = a \cdot T_{s}^i + b$$  \hspace{1cm} (3.3)

It includes LW radiation, because it is usually linearized in BES, with radiant transfer coefficients calculated for each time step in BES.

In Figure 3.6, only the fluxes regarding the interior surface are represented, but in reality, one equation is calculated for each surface (interior and exterior), for each time step in BES.
In this thesis, the flux equation form is adopted in coupling protocols B and C, due to its applicability to a wider range of BEHAM programs. In spite of its limitations, the integrated flux is adopted in coupling protocol A due to its common use in the literature. The coupling variables can be exchanged between the programs in several modes, which are described in the next section.

3.6 Coupling mode

The term coupling mode is introduced in this thesis to describe the sequence used to run programs during the coupling. The coupling mode has usually been considered as part of the coupling strategy (Zhai 2003, Djunaedy 2005, Trcka 2008), which is described in the next section. However, the separation is beneficial to highlight the importance of the coupling mode in coupled simulations. Two possibilities are available:

- One-way coupling (also referred as uni-directional, static or decoupled).
- Two-way coupling (also referred as bi-directional, dynamic or run-time).

In one-way coupling, one of the programs performs a stand-alone simulation and its results are used as boundary conditions or input by the other program. Here, there is no interaction on time step bases. In two-way coupling, both programs run simultaneously and information is exchanged on time step bases during the simulation. Both modes are represented in Figure 3.7.

**Figure 3.7. Coupling modes**

One-way coupling is usually a straightforward technique for a first investigation of the coupling between two programs. It allows a large range of tests, particularly for coupling variables. However, in most real applications there is feedback between the domains modelled in each program. Hence, it is usually necessary to adopt two-way coupling. In this thesis, both approaches are used in different protocols, in order to demonstrate their capabilities and deficiencies. One-way coupling is adopted in protocols A and B. Two-way coupling is adopted in the coupling protocol C, and in this
case it is necessary to define a strategy to exchange coupling variables during their execution. The options of coupling strategy are discussed in the next section.

3.7 Coupling strategy

In cases where two-way coupling is adopted, there are several strategies to exchange variables on time step bases. A more general description divides these strategies into two groups (Hensen 1995, Zhai 2003, Djunaedy 2005, Trcka 2008), which are illustrated in Figure 3.8:

- Strong coupling (also referred to as onion coupling, fully dynamic coupling).
- Loose coupling (also referred to as ping-pong coupling, quasi-dynamic coupling, non-iterative coupling).

In strong coupling, programs exchange information until they reach convergence, while in loose coupling there is no convergence check.

**Figure 3.8. Coupling strategies**

Previous works on coupling have demonstrated the computational benefits of the loose coupling strategy, even with short time step values required to avoid large errors and instability (Trcka et al. 2009). Loose coupling can be performed in two forms, schematically represented in Figure 3.9:

- Parallel execution.
- Sequential execution.

In parallel execution, both programs run simultaneously, and exchange data at a predefined time. It means that at time \( t=2 \), both program will use as boundary condition values calculated by the other program at time \( t=1 \). In sequential execution, only one program runs at a time, while the other waits until it receives information from
the first one. In this case, program 2 will use at time \( t=2 \) boundary condition values calculated by program 1 also at time \( t=2 \). Sequential execution tends to be more stable and accurate than parallel execution; however, parallel execution is faster and shorter time steps can be used to correct oscillations and/or instability.

Sequential loose coupling

**Figure 3.9. Options for loose coupling execution**

In this thesis, a loose parallel coupling strategy is adopted in the coupling protocol C. It is therefore necessary to define a convenient time interval for data exchange (coupling frequency) to preserve stability and accuracy, which is addressed in the next section.

### 3.8 Coupling frequency

Combining the capabilities of BES and BEHAM programs raises temporal and spatial issues. In particular, wind-driven rain presents a challenge, as described in Janssen et al. (2007). The time scale of heat transfer in building elements calculated by BES programs has the order of one hour, while rain absorption by porous materials has the order of seconds.

In BES programs, the time step length is often defined based on previous case studies, rather than on time step independence tests for each case. Previous work indicates that one hour is a good trade-off between accuracy and computational effort in BES simulation (Clarke 2001), and it is also the resolution of most weather data available in CBPS programs (Crawley et al. 1999). It is known that the accuracy of BES simulation depends on the wall composition and node distribution. Nonetheless, using adaptative time steps is not common in BES.

In BEHAM programs, the use of an adaptative time step is more common, particularly due to the necessity of convergence between the coupled system of equations for HAM transfer. The time step can vary from one hour to a few seconds depending on the boundary conditions, particularly when liquid water boundary conditions are applied.
Considering the limitation of BES programs in terms of time step independence, the definition of the data exchange frequency in BES-BEHAM coupled simulations cannot be performed based on general rules. However, values obtained from case studies can be considered as an initial indication for the definition of data exchange frequency in other simulations. The best practice is to test the sensitivity of the simulation results to the data exchange rate value. Results of some of these tests are presented in Chapter 4, and based on them a fixed time step of 6 minutes is used as the initial value in BES ($\Delta t^{BES}$) for two-way coupling in this thesis. The time step in the BEHAM program ($\Delta t^{BEHAM}$) is adaptative, so BES and BEHAM work at different rates (multi-rate) as schematically represented in Figure 3.10. Checks of $\Delta t^{BES}$ time-step independence are performed for all simulations using two-way coupling. In case of one-way coupling, hourly data is exchanged between BES and BEHAM. Independent of the coupling frequency, it is necessary to use computational techniques to exchange the information between programs. These techniques are discussed in the next section.

![Coupling frequency diagram](image)

**Figure 3.10. Coupling frequency**

### 3.9 Inter-process communication

Inter-process communication (IPC) is a purely computational issue in coupled simulations. However, its importance extends from basic aspects such as the time consumed by the simulations to more general aspects, such as the dissemination of coupled simulations. In one-way coupling, IPC is rather simple, usually consisting of text files exported by one program, post-processed and then imported by the other program. However, in cases where two-way coupling is applied, IPC constitutes a main part of the implementation efforts and running time.

Previous studies about coupling mainly used platform-dependant IPC with coding specifically adapted for a particular CBPS program (Djunaedy 2005, Trcka 2008). These
codes are hard to reuse by other users, therefore they are rarely included in new releases of the programs used in the coupling. In order to avoid this situation, a platform-independent IPC with low possibilities of hardcoding was adopted in the current project.

One important option in IPC for CBPS coupled simulation is the Building Controls Virtual Test Bed (BCVTB). It is a “modular, extensible, open-source software platform that allows designers, engineers and researchers of building energy and control systems to interface different simulation programs.” (Wetter and Haves 2008). On the one hand, BCVTB introduces relevant improvements in the dissemination of coupled simulations. On the other hand, BCVTB does not overcome an important limitation on the development of coupled simulation, i.e. the fact that a developer must singlehandedly master both programs. Therefore, BCVTB is not used in this thesis.

In order to overcome some limitations of BCVTB, it was decided to adopt a more traditional approach in the present work, using a small TCP/IP sockets library written in C language, which is compiled with each program, and thus allows their communication during the simulation. Once the coupling protocol is defined, different developers with different areas of expertise can implement the necessary modifications in their codes to perform the coupled simulation. This approach also allows multiple users to run each of the programs involved in the simulation from different computers.

3.10 Coupling protocols

In this chapter, several features of coupled BES-BEHAM simulation were discussed. Each feature can be addressed in several different ways, hence the coupling can be also performed in numerous different ways. This led to the development of various possible coupling protocols. Table 3.1 describes the three coupling protocols used in this research.

Protocol A, from now on also referred to as “one-way coupling using interior air states”, is the most straightforward way of coupling between BES and BEHAM. However, it adopts major simplifications, such as using one-way coupling and neglecting SW and LW radiation from/to surfaces of building elements facing the internal domain. Nevertheless, research has shown that, in some specific cases, it can be used to improve BEHAM calculations (Moon 2005), and that is the motivation to include this protocol in the current research.

Protocol B, from now on also referred to as “one-way coupling using flux equation”, uses a selection of features designed to improve BEHAM calculation based on
detailed boundary conditions from BES results. However, it is not applicable to cases where the whole-building HAM simulation is required, because the final result consists of BEHAM simulations and therefore it can only predict PIs related to building elements.

Table 3.1. Coupling protocols

<table>
<thead>
<tr>
<th>Protocol</th>
<th>Interface node</th>
<th>Domain overlap</th>
<th>Geometrical features</th>
<th>Variables</th>
<th>Mode</th>
<th>Strategy</th>
<th>Maximum frequency</th>
<th>IPC</th>
<th>Controller</th>
<th>Code modification</th>
<th>Pre and Post processing</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Interior air node</td>
<td>-</td>
<td>-</td>
<td>Interior air state</td>
<td>One-way BES BEHAM</td>
<td>-</td>
<td>1 h</td>
<td>Text files</td>
<td>-</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>B</td>
<td>Interior and exterior building element surface nodes</td>
<td>-</td>
<td>1D-1D</td>
<td>Flux equation</td>
<td>One-way BES BEHAM</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>Yes, small</td>
<td>-</td>
<td>No</td>
</tr>
<tr>
<td>C</td>
<td>Interior and exterior building element surface nodes</td>
<td>Supres.</td>
<td>1D-1D</td>
<td>Two-way Loose Paral.</td>
<td>6 min Sockets BES</td>
<td>Yes, large</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

- these features do not apply in this protocol

Protocol C is schematically represented Figure 3.11. This protocol, from now on also referred to as "two-way loose coupling", uses a selection of features designed to explore most of the capabilities of BES and BEHAM programs, while not introducing radical modifications in their codes. In Table 3.1, BES is defined as the controller for the coupling, i.e. the program in charge of starting the simulation and calling the second

Figure 3.11. Scheme of coupling protocol C: Two-way loose coupling
program. Table 3.1 also indicates this is the protocol which demands the larger modifications in the codes. In all the protocols, the programs do not shared pre or post processing.

### 3.11 Conclusions

The discussion about coupling features presented in this chapter allows the following conclusions to be made:

- When compared to the synchronization of the overlapped domain, the suppression of the overlapped domain in the BES program is the best alternative to solve the domain overlap problem.

- Regarding the geometrical resolution, 1D heat and moisture calculation in both BEHAM and BES is the simplest approach to perform BES-HAM coupled simulations.

- 2D and 3D simulations in the BEHAM program coupled with BES would depend, among other factors, on improvements of the convective transfer coefficients in BES. Therefore, it should preferably be carried out when coupling with CFD is available.

- The use of surface discretization to improve the geometrical resolution in stand-alone BES programs presents drawbacks related to the empirical relations for transfer coefficient calculation. Therefore, it should preferably be carried out when coupling with CFD is available.

- Concerning the coupling variables, the BEHAM program should be responsible for the calculation of the states of the boundary nodes, because BEHAM is able to calculate these states taking into account the coupled HAM transport.

- Considering that BEHAM should calculate the states of the boundary nodes, Neumann boundary condition should be used in the BEHAM program, and Dirichlet boundary condition in the BES program.

- Based on literature review and the physical phenomena involved, multi-rate loose coupling with parallel execution seems to be the most suitable coupling strategy.

The next chapter addresses the implementation of the coupling protocols in prototype computer programs using ESP-r and HAMFEM.
3. Coupling protocols
4

Prototype computer programs and verification

4.1 Introduction

In the previous chapter, three coupling protocols were defined, of which two demand modifications in ESP-r and HAMFEM codes for their implementation:

- One-way coupling using flux equation (Protocol B).
- Two-way loose coupling (Protocol C).

This chapter discusses the main changes made in ESP-r and HAMFEM codes to implement these prototypes. It also addresses the verification performed in each implementation.

Coupling protocol A (One-way coupling using interior air states) does not require any modifications in ESP-r and HAMFEM codes. Therefore, this protocol is not discussed in this chapter.

4.2 One-way coupling using flux equation (Protocol B)

The implementation of Protocol B did not demand major modification in ESP-r and HAMFEM. The flow information of this protocol is illustrated in Figure 4.1, where the main modifications can be identified:

- Facility in ESP-r to export flux equations.
- Implementation in HAMFEM of flux equations as boundary conditions.

![Figure 4.1. Scheme of implementation of one-way coupling using flux equations](image)
4. Prototype computer programs and verification

4.2.1 Modifications in ESP-r

The implementation of a facility to export flux equations from ESP-r was divided into two parts, one for heat and one for moisture. Concerning air transfer, it has not been addressed in this implementation, because the only necessary value for one-way coupling (air pressure inside building zones) can be obtained directly from the ESP-r post-processing module.

Regarding the heat flux, the equation for a certain building element has the general form of Eq. (4.1), where $Q_L^t$ is the heat flux for the surface $L$ of the building element at the time $t$ (W), $L$ indicates the surface position (interior or exterior), $a_L^t$ is the linear coefficient, $T_{s_L}^t$ is the surface temperature (K) and $b_L^t$ is the term independent of $T_{s_L}^t$.

$$Q_L^t = a_L^t \cdot T_{s_L}^t + b_L^t \quad (4.1)$$

As described in Section 3.5 and illustrated in Figure 3.6, Eq. (4.1) is composed of several terms representing different heat transfer mechanisms. Eq. (4.1) can be expanded into Eq. (4.2) and Eq. (4.3) for the interior and exterior domains respectively:

$$Q_i^t = Q_{SW-i}^t + Q_{cg}^t + Q_{hvac}^t + h_{ci}(T_{ai}^t - T_{si}^t) + \Sigma(h_{r_{i,n}} T_{sn}^t) - \Sigma h_{r_{i,n}} T_{si}^t \quad (4.2)$$

where $Q_i^t$ is the heat flux for the interior surface at time step $t$ (W/m²), $h_{ci}$ is the convective heat transfer coefficient of the interior surface of the building element (W/m²K), $T_{ai}^t$ is the indoor air temperature (K), $T_{si}^t$ is the interior surface temperature of the building element (K), $h_{r_{i,n}}$ are radiant heat transfer coefficient of the building element to the $n$ surrounding surfaces and $T_{sn}^t$ are the surface temperatures of the $n$ surrounding surfaces (K).

$$Q_e^t = Q_{SW-e}^t + Q_{LWS-e}^t + Q_{LWB-e}^t + Q_{LWG-e}^t + h_{ce}(T_{ae}^t - T_{se}^t) \quad (4.3)$$

where $Q_e^t$ is the heat flux for the exterior surface at time step $t$ (W/m²), $h_{ce}$ is the SW radiation (W/m²), $h_{LWS-e}$, $h_{LWB-e}$, $h_{LWG-e}$ are the LW radiation exchange with the sky, surrounding buildings and ground respectively (W/m²), $h_{ce}$ is the convective heat transfer coefficient of the exterior surface of the building element (W/m²K), $T_{ae}^t$ is the exterior air temperature (K).

By isolating the terms depending on $T_{si}$ and $T_{se}$ in Eq. (4.2) and Eq. (4.3), the coefficients $a_i^t$ and $b_i^t$ of Eq. (4.1) can be obtained (Eq. (4.4) to Eq. (4.7)).

$$a_i^t = -h_{ci} + \Sigma h_{r_{i,n}} \quad (4.4)$$

$$b_i^t = Q_{SW-i}^t + Q_{cg}^t + Q_{hvac}^t \cdot T_{ai}^t + \Sigma(h_{r_{i,n}} \cdot T_{sn}^t) \quad (4.5)$$

$$a_e^t = -h_{ce} \quad (4.6)$$

$$b_e^t = Q_{SW-e}^t + Q_{LWS-e}^t + Q_{LWB-e}^t + Q_{LWG-e}^t \cdot T_{ae}^t + \Sigma h_{r_{i,n}} T_{sn}^t - \Sigma h_{r_{i,n}} T_{si}^t$$
\[ b_e^t = Q_{SW}^t + Q_{LW}^t + h_{ce} T_{ae}^t \] (4.7)

These flux equations consider the whole-building heat balance at each time step. In order to carry out one-way coupling using flux equations, a stand-alone ESP-r simulation is performed and then the calculated values of a and b for the selected building element are written in time step bases into a text file. Figure 4.2 shows the ESP-r interface implemented as part of this thesis to enable the facility to export flux equations.

Concerning the moisture flux equation, the equation for a certain building element has the general form of Eq. (4.8), where \( G_L^t \) is the moisture flux for the surface \( L \) of the building element at the time \( t \) (kg/m²s), \( c_L^t \) is the linear coefficient, \( W_{SL}^t \) is the surface partial vapour pressure (Pa) and \( d_L^t \) is the independent term.

\[ G_L^t = c_L^t \cdot W_{SL}^t + d_L^t \] (4.8)

As opposed to the heat flux equation, the moisture equation has only one term, related to the convective mass transfer. Coefficients \( c_L \) and \( d_L \) are as follows:
where $h_m$ and $h_m$ are the convective mass transfer coefficient (kg/m$^2$ Pa s), calculated based on the analogy with the convective heat transfer (Chilton and Colburn 1934) and $W_a$ is the air partial vapour pressure (Pa). It is known that this analogy is valid in strict conditions (Steeman et al. 2009), and that the use of CFD should be considered when more precise coefficients are necessary (Mirsadeghi et al. 2009, Steeman et al. 2009).

### 4.2.2 Modifications in HAMFEM

In HAMFEM, the only modification required to perform one-way coupling was the implementation of the boundary condition provided by ESP-r. As discussed in Section 2.6, boundary conditions in HAMFEM are implemented directly in the source code for any simulation, therefore the implementation of the flux equations from ESP-r is a straightforward procedure. Flux equation coefficients are included in the HAMFEM standard boundary condition file, which usually provided values of weather data and indoor air states. The subroutine “boundaryconditions” uses the coefficients to calculate the Neumann boundary condition for each iteration.

In this implementation, HAMFEM includes the wind-driven rain load ($G_{WDR}$) at the boundary condition provided by ESP-r. Hence, the moisture flux equation for the exterior domain assumes the form of Eq. (4.13). This approach was adopted because ESP-r has no database for catch ratios, while HAMFEM includes detailed data concerning this parameter (Blocken and Carmeliet 2004, Janssen et al. 2007).

$$G_e = c_e \cdot W_{se} + d_e + G_{WDR}$$  \hspace{1cm} (4.13)

### 4.2.3 Verification

The verification of the implementation of one-way coupling using flux equations was performed using results for the west wall of the BESTEST case 600 building, which has the same geometry, U-values, glazing specifications and heating and cooling set-points as used in the case 900 (heavy-weight - Figure 1.2), and differs only in the thermal capacity.

In ESP-r, the simulations were carried out with no warm-up period, in order to keep simulations consistent with HAMFEM, which has no support for warm-up. ESP-r
usually averages the results over two time steps, while HAMFEM reports the results with no averaging. Again, for consistency, the averaging was disabled in ESP-r.

In all tests, a similar 1D mesh based on the default ESP-r mesh was used in both programs, and is represented in Figure 4.3. ESP-r uses control volumes, i.e. the calculation is performed for volumes in the wall instead of nodes, while HAMFEM uses finite elements, i.e. the calculation is performed for nodes in the wall instead of volumes. These differences could compromise the verification, therefore grid sensitivity tests were performed in both programs. Calculations were performed with the grid illustrated in Figure 4.3 (default ESP-r grid) and with a grid with twice as many cells. Differences in the interior surface temperature in ESP-r were negligible for most of the year (below 0.1°C), therefore the default ESP-r grid was used in the verification. The time step was kept constant in all simulations and is equal to 1 hour. It is known that large time steps can affect BES and BEHAM results; however the focus of this section is on the verification of each implementation and not on the accuracy of the results, addressed in Chapter 5.

4.2.3.1 Verification of ESP-r facility to export the flux equation

The facility to export flux equation in ESP-r was verified by confronting the results obtained with this new facility with standard outputs from ESP-r. Using surface temperatures from ESP-r output (Ts) and exported heat flux equations (a and b), it was possible to calculate integrated heat fluxes (Q) at the interior and exterior surfaces for each time step. These fluxes were compared with hourly values for the flux at the surface (Q'), also obtained using ESP-r post-processing module, as schematically represented in Figure 4.4. The comparison showed no difference between Q and Q'.
4. Prototype computer programs and verification

and thus this implementation is correct and therefore verified. A similar approach was used to verify the implementation to export the moisture flux equations.

**Figure 4.4. Scheme of verification of ESP-r facility to export flux equation**

4.2.3.2 Verification of HAMFEM implementation to use the flux equation from ESP-r

The verification of HAMFEM implementation to use the flux equation from ESP-r was concentrated on the heat transfer equations. The implementation was verified by confronting HAMFEM results with standard outputs from ESP-r. In cases where only heat transfer is calculated, both programs solve the same set of equations based on the Fourier law. Therefore, HAMFEM calculation with boundary conditions from ESP-r heat flux equations should provide surface temperatures (Ts) very similar to the ones calculated by ESP-r stand-alone (Ts’), as represented in Figure 4.5.

**Figure 4.5. Scheme of verification of heat transfer in coupling protocol B**

Figure 4.6 shows a comparison of HAMFEM and ESP-r results in the form of a probability density plot. This figure shows the differences found between the calculated interior surface temperatures by both programs. As expected, the difference is negligible for most of the cases (up to 1.2°C in extreme cases). This difference can be attributed to differences in the numerical methods adopted by each program. Results in Figure 4.6 indicate that the implementation is correct and therefore verified.
Figure 4.6. Comparing ESP-r and HAMFEM results – Interior surface

Figure 4.7. Comparing ESP-r and HAMFEM results – Exterior surface

Figure 4.7 shows the comparison of ESP-r and HAMFEM results for the exterior surface temperature. As in Figure 4.6, the differences are negligible for most of the cases, i.e. approximately 80% of the cases show differences below 2°C. However, some large discrepancies occur in a small range of hours. Figure 4.8 exemplifies one of the situations where these discrepancies can be observed (hours 138 and 160). In these hours, HAMFEM shows a higher variation in the temperature when compared to ESP-r. In HAMFEM, this variation takes place before the corresponding variation in ESP-r. The shift might indicate that the time step adopted can influence the comparisons of results. Indeed, the temporal and special discretization adopted in the simulations can amplify differences related to the numerical methods adopted in ESP-r and HAMFEM. However,
this influence does not compromise the verification. Figure 4.7 and Figure 4.8 demonstrate that ESP-r and HAMFEM results are equivalent, indicating that the implementation of one-way coupling is correct and therefore verified.

![Figure 4.8](image)

**Figure 4.8.** Comparing ESP-r and HAMFEM results – Exterior surface (winter)

### 4.3 Two-way loose coupling (Protocol C)

The implementation of this protocol demanded major modifications in ESP-r and HAMFEM, which are summarized below:

- Facility in ESP-r to export flux equations.
- Implementation of flux equations as boundary condition in HAMFEM.
- Implementation of IPC.
- Improvements in HAMFEM input data and prompt line facility.
- Suppression of the overlapped domain in ESP-r.
- Inclusion of moisture flux from/to wall in ESP-r air node balance.

The first two items from this list were already implemented and verified in the one-way coupling using the flux equations prototype (Section 4.2.3). The other items are addressed in the following sub-sections.

#### 4.3.1 IPC

IPC plays an important role in coupled simulations. As discussed in Section 3.9, TCP/IP sockets in C language are used in this prototype. Implementation of sockets can be demanding due to some specificities of this protocol. There are several sample codes
available in the literature, for both servers and clients using sockets (Stevens 1998). However, a low-level sockets library of functions suitable for coupled simulations in CBPS simulations was not available. Therefore, this library was developed as part of the work described in this thesis based on samples available in literature.

The low-level sockets library intends to facilitate the implementation of communication between CBPS programs using sockets, so this IPC can be implemented by programmers with minimum knowledge of TCP/IP sockets. This library encapsulates in a few subroutines the specificities of this communication protocol, such as: general commands to data format conversion and error handling, as well as standard sockets commands with no importance for final users such as “bind” and “listen”. The library, reproduced in Appendix A, comprises five routines: open server, open client, write, read and close.

The IPC implementation in ESP-r and HAMFEM can be divided into four stages: enable flags and communication addresses for coupling when calling the program in the command prompt, initialization, main loop, and finalization. The first stage is only important for the client program, in this case HAMFEM. The call of HAMFEM in the command prompt must be followed by input data provided by the server program, i.e. port number and the server name (or IP address). In the initialization, a socket is open for each coupled building element and this socket will remain open during the whole simulation, instead of opening and closing sockets inside the simulation loop. In the main simulation loop, the functions “write” and “read” are always used alternately; hence, one of the programs will only send new information after receiving the delivery confirmation from the other program, thus assuring synchronization between them. In the finalization, sockets are closed and the coupling is terminated. These four stages and the use of the low-level sockets library made the implementation of IPC very clear and straightforward, with minimum interference in the code.

4.3.2 Modifications in HAMFEM

The implementation of two-way coupling in HAMFEM demands modifications of some basic features of HAMFEM, which were not necessary in the case of ESP-r. This need is mainly justified by differences in the development time of HAMFEM and ESP-r. ESP-r has more than three decades of active development while the development of HAMFEM began less than 10 years ago. This difference in development time is reflected in a number of facilities and quality assurance procedures that are available in ESP-r but not in HAMFEM. ESP-r, for example, has a sophisticated procedure to assure the quality
of individual contributions to the source code repository. In contrast, there is no repository for HAMFEM developments, and developers share their codes by private correspondence. ESP-r has graphical and text mode interfaces for pre and post-processing and several routines to check the quality and consistence of input data. In HAMFEM, simulations are performed directly from the software development environment (Compaq Visual Fortran), most of the input information has to be modified directly in the source code and there is no check on the input data quality and consistence. Therefore, a number of modifications were implemented in HAMFEM in order to bring it to the level necessary to perform two-way coupled simulations. These modifications consisted of:

- Removing hardcoded information.
- Creating a prompt line facility.
- Removing limitations in file names and paths.

The original HAMFEM code had much input and boundary condition information hardcoded, i.e. implemented directly in the code instead of in input text files. Due to this characteristic, it was necessary to modify the code for every simulation. Considering that verification and validation must be carried out every time that the code is modified, it is virtually impossible to verify and validate the original HAMFEM code for general purpose use. Concerning this issue, HAMFEM was modified to provide a number of predefined boundary conditions that can be selected using default input text files. Moreover, all input information was externalized and it is now available in text files, such as material properties database, location latitude, and solar absorptivity.

Once the hardcoded information was removed from the source code, it was possible to compile a general purpose HAMFEM executable. In order to obtain some flexibility in the use of this executable, a number of restrictions in the original code had to be removed, such as restrictions to folder names, restriction to file names and information provided in parts of file names. Moreover, a prompt line facility was developed to inform the program about input file names and, in case of external coupling, the address for communication with ESP-r.

### 4.3.3 Modifications in ESP-r

The modifications in ESP-r code affected the core of its calculation engine. The complexity and extension of modifications necessary to perform a coupled simulation seem to be proportional to the code size and history.
Two major modifications were implemented in the main module of ESP-r: (a) extraction of the flux equation for the surfaces of each coupled building element (as described in Section 4.2.1); and (b) suppression of nodes from the ESP-r matrix corresponding to the coupled building element. This section provides high level information about the implementation to suppress nodes from the ESP-r matrix, and Appendix D provides a more detailed description of the files modified in ESP-r code.

As discussed in Section 3.3, conflicts due to the domain overlap between BES and BEHAM programs can be overcome by the suppression of overlapped nodes from one program. In ESP-r, a single matrix simultaneously solves the heat transfer for each zone, including all building element nodes and the indoor air node, as schematically represented in Figure 4.9. Although all nodes are solved simultaneously, ESP-r is very suitable for the suppression of the overlapped domain, due to the procedure adopted to form and solve the heat balance matrix. This matrix is partitioned into several matrices, one for each building element \( W_n \) and one for the interior air and interior surface nodes \( R \). Due to this partitioning, the suppression of one building element does not affect the matrices of other building elements. The building element matrices are coupled with the matrix for the air and surfaces nodes, and only this matrix had to be modified for two-way coupling simulations.

Figure 4.9 . Scheme of ESP-r nodes and connections for a zone (Clarke 2001)
In the interior air and interior surface nodes matrix - \( R \), the surface temperature of the coupled building element is known (calculated by HAMFEM), so its equation had to be removed from this matrix. Some terms related to the heat exchange between the coupled surface and the surrounding surfaces were calculated by multiplying the known surface temperature with the corresponding coefficients in the matrix, where the result is transported to the right-hand side of the matrix, as represented in Figure 4.10.

Figure 4.10 shows the air and surface nodes matrix at time equal to \( t+1 \). Assuming that the first line represents the coupled building element, this line was suppressed from the matrix, as well as the columns with the cross-coupling coefficients relative to this building element (first 2 columns), resulting in the matrix indicated in gray/magenta. For each one of the remaining nodes, the cross-coupling coefficients related to the coupled building element were multiplied by the surface temperature at time equal to \( t \), as calculated by HAMFEM, and transported to the right-hand side of the equation. This concludes the implementation related to heat transfer in ESP-r.

Concerning the moisture terms, the modifications in the code were much smaller. The only relevant modification was the inclusion of the moisture flux from/to the building element into the air node moisture balance. This flux was calculated using the surface vapour pressure calculated by HAMFEM and mass transfer coefficients obtained using the analogy with heat transfer coefficients calculated by ESP-r.

One important limitation of the current implementation is the impossibility of placing control/sensor nodes in the coupled building elements. Concrete core activation and other techniques in which there is heat injection/extraction inside the building element cannot be simulated using this coupling protocol.

Another important, but rather philosophical, aspect of the current implementation is the disassembling of the ESP-r core. In the case where all the
building elements are coupled with HAMFEM, the only node remaining in ESP-r calculation is the air node. One might argue that in this case, ESP-r is reduced to a sophisticated pre and post-processor for the BEHAM program. In fact, many of the ESP-r qualities are based in pre and post-processing, and also in the integration with other domains, such as AFN, HVAC system, CFD, renewable energies, etc. In this sense, much of the power of ESP-r is preserved in the present coupling protocol.

It is clear that ESP-r stand-alone is highly optimized for 1D calculations of heat transfer in building elements, and that the current prototype cannot compete in terms of computational efficiency for problems involving only heat transfer.

### 4.3.4 Verification

Several measures were adopted to verify the implementation of the coupling protocol described in the previous sub-sections. Considering the complexity involved in any kind of coupling, it is advisable to perform the implementation and verification in steps. In most verification exercises, the BESTEST case 600 building was used, and the four walls, floor and ceiling were simulated using two-way loose coupling. Initial conditions were fixed to 15°C and 50% RH (unless indicated differently in a specific test). The simulations were carried out for one year, and data exchange frequency was fixed at 6 minutes.

The next three sub-sections describe the verification of IPC, modifications in HAMFEM and in ESP-r.

#### 4.3.4.1 Verification of IPC

The low-level sockets library is verified by its implementation in two programs designed to emulate ESP-r and HAMFEM. These emulators (see Appendix B) act as a server and a client exchanging predefined information (fixed or variable), and they have a threefold importance. Firstly, they allow the verification of the low-level library by the comparison of values sent by one program and received by the other (Figure 4.11 - Phase 1). Secondly, they provided the means to test the compilation of this library and its use in different operational systems and machines (Figure 4.11 - Phase 1). During this research, for example, it was necessary to compile and test this library on several systems (Solaris, Linux 32-bits and Linux 64-bits) and machines (using Spark and x86 processors). Thirdly, these emulators can be used to separately test ESP-r and HAMFEM implementations of two-way coupling (Figure 4.11 - Phase 2). In all cases, the verification in the IPC is straightforward, because it consists only of the comparison of
values sent by one program and received by the other. The tests described in phases 1 and 2 of Figure 4.11 were performed and showed identical values (sent and received), and thus the IPC was verified. Phase 3 shown in Figure 4.11 is designed to test the whole prototype implementation (see Section 4.3.4.4). In this case the focus is not on IPC, which was previously verified, but on the other coupling features implemented in HAMFEM and ESP-r.

4.3.4.2 Verification of extensive code rearrangement in HAMFEM

The main modification in HAMFEM was an extensive code rearrangement to improve data input and prompt line facilities. The verification of this implementation was carried out using a test suite developed in this thesis to assure the quality of new contributions to the HAMFEM code.

The new test suite is composed by a program (Hamfem-tester) that automatically runs several simulations in HAMFEM and compares results of new code against benchmark results generated by the original and validated code. The comparison is performed for all nodal states in HAMFEM output files, and the differences are summarized in a table with their minimum, maximum, mean and RMSE values. The test comprises five cases: steady state moisture transfer; atmospheric boundary conditions with wind-driven rain; atmospheric boundary conditions without wind-driven rain; HAMSTAD exercise 1 and HAMSTAD exercise 4. After each modification carried out in HAMFEM code during the development of this thesis, the test was performed again assuring that the new code produced results as good as those obtained with previous versions of HAMFEM. Compared to the ESP-r test suit, HAMFEM-tester has a large space for improvements. However, it provides minimum quality assurance in the developments carried out in this thesis.

Figure 4.11. Scheme of IPC emulators and verification
4.3.4.3 Verification of the suppression of overlapped domain in ESP-r

The level of modifications in ESP-r for the suppression of overlapped domain makes its verification a fundamental step in the implementation of two-way coupling. This verification was performed using results of stand-alone ESP-r to test the new implementation. In this thesis, this approach is referred to as self-coupling and is schematically represented in Figure 4.12.

![Figure 4.12. Scheme of verification of suppression of overlapped domains](image)

In Figure 4.12, two results are extracted from stand-alone ESP-r: a PI such as the annual cooling energy demand ($E'$) and hourly surface temperature values for a certain building element ($Ts'$). These surface temperature values are implemented in a client emulator, which plays the role of HAMFEM sending $Ts'$ to ESP-r. The simulation using the client emulator should produce the same value for the performance indicator ($E$) as the stand-alone simulation ($E'$). Results were compared and showed no differences, and consequently this implementation was verified.

4.3.4.4 Verification of the whole prototype for two-way loose coupling

The verification of the whole prototype was divided into two parts, one for heat and one for moisture. Considering that the implementation related to heat is more complex than the one related to moisture, most of this section is dedicated to the verification of whole-building heat transfer using two-way loose coupling. In cases where only heat transfer is taken into account, both ESP-r stand-alone and the two-way loose coupling prototype solve the same set of equations, they should consequently produce the same results. For this reason, ESP-r stand-alone is used in this section as a source of reference data to verify the two-way loose coupling prototype concerning heat.
4. Prototype computer programs and verification

The verification for heat consists of three parts. Initially, surface temperatures were compared. This was followed by comparisons of heating and cooling energy demand and peak power demand for a building with HVAC system. Finally, comparisons of interior air temperature in buildings with neither heating nor cooling were carried out. These three parts are described in the next paragraphs.

Surface temperatures are important for the evaluation of condensation and mould growth risk, therefore the verification starts with an exercise focused on this PI. As in Section 4.2.3, this exercise uses the west wall of the BESTEST case 600 (Figure 1.2). However, the time step adopted in the present section for ESP-r simulations is reduced to 6 minutes. This reduction avoids oscillations in the surface temperature results that can be observed even in ESP-r stand-alone, as exemplified in Figure 4.13. It is important to stress that in this coupling protocol, the data exchange frequency is defined by the BES time step, therefore reductions in ESP-r time step also increase the data exchange frequency, reducing inaccuracies related to the use of loose coupling.

![Figure 4.13. Oscillation in ESP-r results for large time steps](image)

The BESTEST case 600 building has eight surfaces, of which six are made of hygroscopic materials (four walls, roof, floor) and two are moisture tight (the windows). Hence, only the six hygroscopic surfaces are coupled and calculated by HAMFEM, while the heat transfer through the windows is calculated by ESP-r. Figure 4.14 shows a comparison of results obtained using ESP-r stand-alone and the two-way coupling prototype, where a good agreement is found. As in section 4.2.3.2, the difference between ESP-r stand-alone and the two-way coupling prototype were presented using histograms. Figure 4.15(A) shows that the differences are mostly restricted to plus or minus 1 °C, which is a clear improvement to one-way coupling results (see Figure 4.7).
Figure 4.15(B) also shows that large differences can eventually be found during a short period, i.e. in cases where a large change in the surface temperature takes place in a very short time interval. Based on results presented in Figure 4.14 and Figure 4.15 the prototype was verified concerning the calculation of surface temperatures. In the next paragraphs, the prototype is verified for the calculation of annual heating and cooling energy demand and peak power demand.

![Graph showing surface temperature over time](image)

**Figure 4.14**. Comparison of ESP-r results and two-way loose coupling results for surface temperature over time

![Graph showing frequency of occurrence and variation over time](image)

**Figure 4.15**. Comparison of ESP-r results and two-way loose coupling results for surface temperature. Frequency of occurrence (A) and example of variation over time (B)

Annual energy demand is a PI that is much more sensitive to the data exchange frequency than surface temperatures, because small errors can lead to large differences when integrated over the year. Hence, an independence check was performed regarding the data exchange frequency for this PI, as shown in Figure 4.16 where the
data exchange frequency is equal to ESP-r time step. The figure demonstrates the strong impact of data exchange frequency, which is more pronounced in cases where more surfaces are coupled. For engineering applications, a time exchange interval of 6 minutes would provide good results for this building and PI. However, the present verification adopted a one-minute interval in order to obtain higher confidence in the comparison.

**Figure 4.16.** Time step independence test using two-way loose coupling

**Figure 4.17.** Verification of using BESTEST 600 and 900 intervals
Figure 4.17 shows the results of energy demand and peak power demand for cooling and heating obtained using the two-way loose coupling prototype. This figure includes results for both the Case 600 and 900, and in both cases the results are very similar to ESP-r stand-alone results and are always in the range prescribed by BESTEST. Based on the results presented in Figure 4.17, the prototype was verified for the calculation of energy demand and peak power demand.

The last exercise for the verification of heat transfer in the prototype was focused on buildings with neither heating nor cooling systems. This exercise used the BESTEST cases 600FF and 900FF, which are identical to the cases 600 and 900, except for the absence of HVAC systems. Figure 4.18 shows the results obtained with the two-way loose coupling prototype, which are in range for five out of six cases. The maximum temperature predicted by the prototype in Case 600FF is slightly lower than the prescribed range, but the difference is negligible. Based on the results presented in Figure 4.18 the prototype was verified for the calculation of temperature in buildings with no HVAC.

![Figure 4.18. Verification of using BESTEST 600FF and 900FF intervals](image)

The previous paragraphs demonstrated the verification concerning heat transfer. The verification of moisture transfer was carried out in a simplified way for two reasons. Firstly, the implementation itself was simple when compared to modifications
necessary for the implementation of heat transfer. Secondly, the first validation exercise (Section 5.2) is dedicated to calculating an analytical solution for isothermal moisture transfer, which by consequence verifies the functionalities related to the solution of this problem. Therefore, the implementation of moisture transfer was tested here using simple sanity tests (Desikan and Ramesh 2007). Sanity tests aim to “test the major behaviour or functionality of the application” (Limaye 2009). The first test evaluates the effect, on ESP-r interior air node, of artificially keeping in HAMFEM a constant humidity in the wall. When the wall is kept saturated in HAMFEM, this wall will provide a large flux of moisture into the interior domain, and the air node in ESP-r should present a large increase in RH. The opposite effect is expected when the wall is kept dry in HAMFEM. Figure 4.19 shows the results of this sanity test by presenting the variation of RH in interior air node in ESP-r for 3 cases: the reference case (ESP-r stand-alone), the case of a dry wall in HAMFEM (where it is possible to see the expected reduction in RH of the interior air node) and the case of a saturated wall in HAMFEM (where it is possible to see the expected increase in RH of the interior air node). This sanity test indicates that the implementation reproduces well general trends. The second sanity test works in a similar way, by artificially keeping ESP-r air node RH in two extreme values and observing the impact of these extreme values in the moisture content of the wall calculated by HAMFEM. Results of this second test are not graphically presented here for brevity, but they also demonstrate that the variation of RH in HAMFEM is consistent with the extreme values defined in ESP-r, indicating that the implementation of moisture reproduces general trends well, and it is verified.

Figure 4.19 . Interior air RH in ESP-r during verification with a sanity test
4.4 Conclusions

The discussion of implementation and verification presented in this chapter allows the following conclusions to be made:

- The implementation of one-way coupling using flux equation (Protocol B) was successfully verified.
- The implementation of two-way loose coupling (Protocol C) was successfully verified.
- IPC using C language socket libraries proved to be easily implemented and flexible in its application.
- Self-coupling proved to be a valuable technique for verification, particularly in BES.
- One-way coupling proved to be a useful technique for verification purposes.
- Emulators proved to be fundamental in the development and verification of coupled simulation programs.
- Comparison of results from coupled simulation with standard outputs of stand-alone simulations proved to be useful for verification.
- HAMFEM and ESP-r proved to be suitable codes for BES-BEHAM coupling. Some of the implemented facilities, such as exporting “surface flux to HAM model”, can be readily used with any BEHAM code.
- Data exchange frequency should be always evaluated by independence tests when two-way loose coupling (Protocol C) is used.
4. Prototype computer programs and verification
5

Validation

5.1 Introduction

One of the basic aspects of science is the development of models to explain and/or predict reality (Kuhn 1970, Bunge 1972), and validation is a key step in the development of models. The term validation has been given different meanings in various technical disciplines (Oberkampf et al. 2004). In this thesis, validation is defined as “the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model” (AIAA 1998). Similarly to other works dealing with coupled simulation (Djunaedy 2005, Trcka 2008), the validation process is carried out by comparing simulation results against reference data, such as from analytical solutions, inter-model comparison and experimental results. Regarding the availability of reference data, the ASHRAE Handbooks provides very clear statements: “Validation, verification, and benchmarking of combined heat, air and moisture models is a formidable task. Currently, only limited internationally accepted experimental data exist” (ASHRAE 2005); “The main difficulty lies in the fact that it is difficult to measure air and moisture fluxes and moisture transport potentials, even under laboratory conditions” (ASHRAE 2005). Based on these two quotes, the validation of whole-building HAM simulation programs, such as the ones developed in this thesis, should be understood as a work in continuous progress, and the results provided in this chapter are an initial demonstration of the current capabilities of coupled BES and BEHAM simulations.

This chapter comprises six validation exercises, which are briefly described below. The first five are dedicated to the two-way loose coupling prototype (coupling protocol C), which is the most comprehensive prototype developed in this thesis. These five exercises have an increasing complexity, starting from an analytical solution of isothermal moisture transfer, followed by three inter-model comparisons with increasing complexity, and finalized by an experimental validation. After the validation of the two-way loose coupling prototype, it is used in the last exercise to validate the simulations.
based on coupling protocol A (one-way coupling using interior air states) and the prototype based on coupling protocol B (one-way coupling using flux equation).

5.2 Analytical solution for isothermal vapour transfer

5.2.1 Problem outline

"In general, it is difficult to develop worthwhile test cases that can be solved analytically or quasi-analytically, but such solutions are extremely useful when possible. An analytical solution provides an exact mathematical truth standard, limited to highly constrained cases for which exact analytical solutions can be derived." (Neymark and Judkoff 2008).

The first step in the validation of the two-way loose coupling prototype was the comparison with two analytical solutions formulated by Thomas Bednar and Carl-Eric Hagentoft (Woloszyn and Rode 2008). Figure 5.1 shows information about the building, assumptions and inputs used in the solutions of moisture balance in the room in isothermal conditions. The analytical solution provides the variation of RH in the zone over time. Moisture is released in the room according to the profile in Figure 5.2 and it is removed from the interior air by a fixed air change rate of 0.5 ACH. Here, only the solution for the \( n^{\text{th}} \) day is reported. Analytical solutions are available for two scenarios: one with no moisture buffering (sealed surfaces) and another with buffering (only outer surface is sealed). In the case with no moisture buffering, the results obtained using ESP-r stand-alone or the two-way coupling prototype are identical (for a time step of 1 minute), therefore only ESP-r results are reported. For the case with moisture buffering, results using two-way loose coupling and using ESP-r stand-alone are reported.

![Diagram of building](image)

**Figure 5.1.** Building used in the isothermal analytical solution of moisture buffering

<table>
<thead>
<tr>
<th>Isothermal (( T_{\text{ref}} = 20 , ^\circ\text{C} ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{RH}_{\text{out}} = 30 % )</td>
</tr>
<tr>
<td>0.5 ACH</td>
</tr>
<tr>
<td>Emissivity ( \equiv 0 )</td>
</tr>
<tr>
<td>SW absorptivity ( \equiv 0 )</td>
</tr>
<tr>
<td>All surfaces face the outside air</td>
</tr>
</tbody>
</table>

Material

Aerated concrete (\( e = 15 \, \text{cm} \))
5.2.2 Results and discussion

Figure 5.3 shows the result for the case with no moisture buffering, where a very good agreement is observed. The results show a continuous increase in the RH during the period with moisture release in the room (from 9:00 to 17:00) leading to a maximum of approximately 73% RH, and after that the RH in the room starts to decrease until it reaches equilibrium with the outside conditions at 30% RH.

Figure 5.4 shows results for the case with moisture buffering, where a very good agreement is observed between the analytical solution and the two-way loose coupling results. Results of ESP-r stand-alone do not take the buffering into account and consequently show large deviations from the analytical solution. It is worthwhile to note that the moisture buffering in this case is rather extreme, reducing the daily variation in RH from about 43% to less than 10%, i.e. buffering of approximately 75% of the daily variation. This means that ESP-r overestimates the amplitude by a factor of 4.
5. Validation

5.3 Inter-model comparison of HAM transfer in a small cube

5.3.1 Problem outline

Analytical solutions for combined heat and moisture transfer at the whole-building level are not available. However, it is possible to use extensively validated and high resolution numerical simulation programs to obtain approximate solutions for a variety of simplified and sometimes even complex problems (Neymark and Judkoff 2008). In this validation exercise, a CFD-HAM model (Steeman et al. 2009) was used to solve a problem of conjugate heat and mass transfer in the solid and fluid domains. The problem under analysis is the propagation of heat and moisture in a small cube where a step function is applied at one of the boundaries, as schematically represented in Figure 5.5. The problem is initialized at 30 °C and 30% RH, one boundary is kept at this condition while the step function is applied at the outer surface at the opposite side of the cube. The other four surfaces are adiabatic. The cube is filled with air and all walls are made of brick with a thickness of 8 cm. Results of temperature and humidity ratio by mass for the first four hours were compared, both for the average indoor air and for the interior surface of the hot wall (surface averaged). This problem is particularly sensitive to the heat and mass convective transfer coefficients, which are generally identified as a significant source of uncertainty in whole-building simulation. For this reason, convective transfer coefficients used in the two-way loose coupling simulations were determined based on the CFD results (Mirsadeghi et al. 2008).
5.3.2 CFD-HAM simulation

The CFD-HAM simulations were carried out using the commercial software Fluent, improved by an internally coupled BEHAM code programmed using user-defined functions (UDFs) (Steeman et al. 2009). The Fluent engine is responsible for the calculation in the fluid domain and for the solution of transport equations defined in the BEHAM code. This BEHAM code describes the coupled heat and moisture transfer in 3D over the whole domain (fluid and all solid elements). In the solid domain, vapour diffusion is taken into account. Figure 5.6 shows the mesh and the main settings used in the present simulations, and also reports some of the best practices in CFD simulations that were followed in this work. The buoyant flow was previously validated using experimental results (Mirsadeghi et al. 2008).

- k-ω turbulence model
- Low-Reynolds modelling (solid-fluid interface)
- Mesh independence tested
- $y^+ < 1$
- Convergence criteria – $10^{-6}$
- Transient simulation
- Time step – 0.5 s
- Heat and mass transfer calculated using a custom code programmed with user-defined function

5.3.3 Results and discussion

Figure 5.7 shows contour plots of the humidity ratio and temperature obtained using CFD-HAM after four hours physical simulation time. For both PIs, the overall
behaviour is in accordance with expectations. It is possible to see the propagation of heat and moisture in the left wall, and its effects in the air volume and in the upper wall. The air volume shows a rather uniform distribution in the humidity ratio, with an average around $9\times10^{-2}$. The temperature varies about 5 °C in the fluid domain with an average around 33 °C, although a small zone with higher air temperature is present in the top of the hot wall.

Figure 5.7. CFD-HAM results of humidity and temperature in a cross section

Figure 5.8 shows the evolution in time of the humidity ratio in the air and in the inner surface of the hot wall, where a good agreement between the CFD-HAM results and two-way loose coupling results can be observed. Figure 5.9 shows the results for temperature, which also show very good agreement. As described before, these results are highly affected by convective heat transfer coefficients, and thus the use of CFD in combination with the two-way loose coupling prototype is advisable.

Figure 5.8. Humidity ratio results
5.4 Inter-model comparison of HAM transfer in a simplified building

5.4.1 Problem outline

The third validation exercise was proposed during the IEA-ECBCS Annex 41 and is summarized here in Figure 5.10. It consists of a one-zone building with the same geometry as the BESTEST building, although some simplifications are introduced in the materials and boundary conditions: (1) the building is not in contact with the ground (all faces in contact with exterior air including the floor, as a building supported by free-standing pillars), (2) only one material is used in all opaque surfaces (aerated concrete), (3) windows have a higher solar heat gain coefficient (equal to 1 in order to simplify the simulation) and (4) the climate file of Copenhagen is used because it is less severe than Denver climate originally used in BESTEST (Woloszyn and Rode 2008). Moisture is released in the building interior according to the profile in Figure 5.2. The results of six PIs over time should be calculated for the day 5th of July. In the original inter-model comparison carried out during IEA-ECBCS Annex 41, 12 different solutions were provided using different whole-building HAM programs. Results show large variations, which raises questions about the validity of using such results as reference for any comparison. Therefore, the results from IEA-ECBCS Annex 41 presented in this thesis were post-processed in two groups, the first is composed of all 12 different solutions (wide range), and the second is composed of only 8 solutions (narrow range), discarding, hour by hour, the two higher and two lower results. In the next section,
these two groups of results from IEA-ECBCS Annex 41 are compared with the solutions obtained using the two-way loose coupling and ESP-r stand-alone. Although this exercise adopts several simplification and do not rely on analytical or experimental data, it is a necessary step in the validation process, which should be carried out in steps of growing complexity in order to allow the identification of possible individual flaws in the program.

Location: Copenhagen, Denmark
Solar heat gain coefficient = 1
Heating set-point = 20 °C
Cooling set-point = 27 °C
0.5 ACH

Material
Aerated concrete (e = 15 cm)
U_{wall} = 1 W/m².K
U_{roof} = 1 W/m².K
U_{window} = 3.0 W/m².K

Figure 5.10 . Simplified BESTEST building used in IEA-ECBCS Annex 41

5.4.2 Results and discussion

Figure 5.11 shows results for the interior air temperature and exterior surface temperature of the roof. These PIs are not strongly affected by moisture transfer through the building envelope, and consequently both ESP-r stand-alone and the two-way loose coupling provide similar results. The results obtained in this thesis agree with the narrow range of results from IEA-ECBCS Annex 41. It is also noticeable that the narrow range of results from IEA-ECBCS Annex 41 indicates good agreement between the 8 solutions for most of the PIs; hence the validity of this inter-model comparison increases significantly.

Figure 5.12 shows the results of energy demand for heating and cooling. As in Figure 5.11, the results are not affected by moisture, i.e. ESP-r stand-alone results are very similar to the two-way loose coupling results. Both results show good agreement with the narrow range. It should be noticed that the agreement between solutions in the narrow range is much better for heating energy demand than for cooling.

Figure 5.13 presents the results for indoor air RH and exterior surface RH of the roof. Due to the moisture buffering, the two-way loose coupling prototype provides results for the indoor air RH that are in much better agreement with the narrow range than ESP-r stand-alone results. For the exterior surface RH of the roof, ESP-r stand-
alone is not able to predict this indicator, so only the two-way loose coupling results are
presented, which are in good agreement with the narrow range. As in Figure 5.11, the
narrow range in Figure 5.13 demonstrates that the apparent variation in the results of
IEA-ECBCS Annex 41 is mainly caused by outliers and in general the 8 central solutions
have good agreement.

![Figure 5.11](image1)

![Figure 5.12](image2)

Figure 5.11. Temperature results of an inter-model comparison for a simplified
version of the BESTEST building, for the day 5th of July

Figure 5.12. Energy results of a inter-model comparison for a simplified
version of the BESTEST building, for the day 5th of July
5. Inter-model comparison of HAM transfer in the BESTEST building

5.5.1 Problem outline

The fourth validation exercise was also proposed during the IEA-ECBCS Annex 41, and is summarized in Figure 5.14 (Woloszyn and Rode 2008). The building used in this exercise is very similar to the original BESTEST case 600 building, except for a few modifications in the thermal capacity (discussed in Section 5.5.2) and in the interior moisture gain, which follows the profile presented in Figure 5.2.

Location: Denver, USA
- \( U_{\text{wall}} = 0.5 \text{ W/m}^2\cdot\text{K} \)
- \( U_{\text{roof}} = 0.3 \text{ W/m}^2\cdot\text{K} \)
- \( U_{\text{window}} = 3.0 \text{ W/m}^2\cdot\text{K} \)
- 0.5 ACH

Solar heat gain coefficient = 0.78
Heating set-point = 20 °C
Cooling set-point = 27 °C
During the IEA-ECBCS Annex 41, 13 different solutions were provided using different whole-building HAM programs for four PIs: heating energy demand, cooling energy demand, heating peak power demand and cooling peak power load. Similar to the previous sections, the results reported in the IEA-ECBCS Annex 41 show very large variations in the results. The next section analyses the differences between the original BESTEST results and the results obtained in the IEA-ECBCS Annex 41, and also provides a narrow range considering 9 out of the 13 solutions reported in IEA-ECBCS Annex 41. Section 5.5.3 reports and discusses the results obtained using the two-way loose coupling prototype.

### 5.5.2 Analysis of results from IEA-ECBCS Annex 41

Figure 5.15 shows a comparison of ESP-r stand-alone results for the original BESTEST case 600 building and for the version of this building proposed by IEA-ECBCS Annex 41. The results demonstrate that the modifications proposed by IEA-ECBCS Annex 41 significantly affect the results, even when moisture transfer is not taken into account, making it difficult to compare results from the original BESTEST with results from IEA-ECBCS Annex 41. Figure 5.16 shows a comparison between dry material properties used in the original BESTEST and in the IEA-ECBCS Annex 41, where large differences in the thermal mass can be observed. Considering the increase in thermal mass in IEA-ECBCS Annex 41, the reduction of all PIs observed in Figure 5.15 is indeed expected, and is consistent with the results from the original BESTEST.

**Figure 5.15.** ESP-r stand-alone results for the BESTEST case 600 building

Figure 5.17 shows the ranges provided by the original BESTEST, by IEA-ECBCS Annex 41 and the narrow range calculated in this thesis using 9 out of 13 solutions. As
in Section 5.4.2, the narrow range shows that the variations in the results in IEA-ECBCS Annex 41 are due to outliers, and that most programs agree with each other. For the case 900, the narrow range is very similar to the original BESTEST, demonstrating that

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**Figure 5.16**. Difference in material properties between the original BESTEST case 600 and IEA-ECBCS Annex 41

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**Figure 5.17**. Comparison of ranges the provided in the original BESTEST and the solutions reported in IEA-ECBCS Annex 41
moisture plays a minor role in the results. The case 600 shows different behaviours regarding heating and cooling. For cooling, the narrow range is slightly larger than the original BESTEST, and it is shifted towards lower values, which is consistent with results from Figure 5.15 as well as with original BESTEST results. For heating, the narrow range is very similar to the original BESTEST, while a shift towards lower values would be expected according to results in Figure 5.15. This could indicate that programs used in IEA-ECBCS Annex 41 overestimate the heating energy demand for this building.

5.5.3 Results and discussion

Figure 5.18 shows the results obtained for the BESTEST case 600 building (as described in IEA-ECBCS Annex 41) using two-way loose coupling. Firstly, it can be observed that most results are in agreement with the narrow range of results obtained using the other 9 CBPS programs. The exception is the heating energy demand, but Section 5.5.2 demonstrated that solutions provided in IEA-ECBCS Annex 41 might overestimate this PI. Secondly, the comparison between results obtained using conjugate heat and moisture transfer and results obtained using only heat transfer indicate that moisture plays a minor role in this particular building and PIs. This fact can, in part, be attributed to the low impact of moisture in the thermal conductivity and thermal mass of this particular case, as shown in Figure 5.19. Moreover, the magnitude of latent heat flux in this building (under this particular weather) is negligible, as shown in Figure 5.20. In Figure 5.20(A), the relation between moisture flux and latent heat is represented (assuming moisture at 20°C). The region highlighted in the figure indicates the range of

![Figure 5.18. Results for the BESTEST case 600 building in IEA-ECBCS Annex 41 using two-way loose coupling](image-url)
values found in the interior and exterior surface of the BESTEST case 600 building using two-way loose coupling. For the interior surface, the values are negligible, while latent fluxes up to 12 W/m² are found at the exterior surface. The fluxes at the external surface are not high when compared to solar radiation, and Figure 5.20(B) indicates that most of the time the latent heat flux at the external surface is in fact much lower than 12 W/m².

![Figure 5.19. Variation in material properties due to moisture](image1)

![Figure 5.20. Relation between latent heat and moisture flux (A) and the frequency of occurrence of different latent heat flux values (B)](image2)

Although moisture accumulation and fluxes do not play a major role in energy demand and peak power demand, the initial conditions of moisture in the wall
significantly affect the results. This effect can be observed in Figure 5.21, where the uncertainty due to moisture initialization is shown in comparison with the range of solutions described in the IEA-ECBCS Annex 41. Firstly, the impact of initialization is noticeable, particularly on energy demand. Secondly, it is possible to explain most of the variation in the different solutions solely by using this parameter.

![Figure 5.21. Uncertainty in the results due to initialization of moisture](image)

### 5.6 Experimental validation of moisture buffering

#### 5.6.1 Problem outline

The last validation exercise focused on the two-way loose coupling prototype investigates the variations in RH and heating energy consumption in experimental rooms at Holzkirchen, Germany (see Figure 5.22) with indoor moisture gains according to Figure 5.23, where a series of measurements was carried out during IEA-ECBCS Annex 41 (Woloszyn and Rode 2008). This exercise only uses the set of measurements

![Figure 5.22. Experimental room in Holzkirchen](image)
in which the interior finishing of the room is composed of painted gypsum plaster. The window is fully covered by an external sheet in order to avoid any SW gain (solar heat gain coefficient equal to 0). In the description of the measurements, there is no information available about the corridor that faces the test room, and the room is described as “thermally decoupled”. There is also no information about measurement uncertainties.

Figure 5.23. Moisture gains profile used in experiments in Holzkirchen

5.6.2 Results and discussion

Figure 5.24 shows the variation of RH during a period of 17 days. Measurements and predictions using two-way loose coupling are in very good agreement most of the time. Differences between measurements and predictions are also plotted in Figure 5.24, and it is possible to see that small delays in the predictions lead to discrepancies of up to 10 % in RH. However, these discrepancies are restricted to only one or two hours per day and are related to small shifts between experimental results and simulation results. Minimum and maximum values as well as the daily amplitude predicted using two-way loose coupling are very close to the experimental results, with slight under prediction.

The results presented in Figure 5.24 are based on a preliminary calibration of the initial moisture content of walls, performed based on the first two days of measurement. The initial moisture content of walls was not described in IEA-ECBCS Annex 41; however, tests using the two-way loose coupling prototype demonstrated that this parameter is very important for the solution of this problem. The discrepancies between solutions presented in IEA-ECBCS Annex 41 are consistent with the variation observed during the calibration of the initial moisture content. Participants of IEA-ECBCS Annex 41 did not have previous access to the experimental results; therefore they could not calibrate their simulations as it was done in this thesis. Other inputs which were
potential candidates for calibration, such as heat and mass transfer coefficient, were not modified for this particular simulation.

Figure 5.24. Variation of relative humidity (17 days period)

Figure 5.25 shows two days of results extracted from Figure 5.24 in order to allow the comparison between ESP-r stand-alone results and two-way loose coupling prototype results. In the figure, the differences between predictions and measurements are also plotted. Although ESP-r reproduces the overall trend in the results, it consistently overestimates the amplitude of daily variations in RH. The ratio between the daily measured amplitude (m) and the calculated amplitude using ESP-r stand-alone (P) is on average 0.62 (Table 5.1). This ratio shows a much larger disagreement than the ratio between daily measured amplitudes (m) and the calculated amplitudes using two-way loose coupling (p) which is on average 1.1 (Table 5.1), i.e. very close to the unity. Discrepancies in the results using two-way loose coupling can be mainly attributed to small shifts between experimental results and the predictions, while the discrepancies in ESP-r results are mainly due to the absence of moisture transfer/buffering models. It can be concluded that the use of two-way loose coupling
provides significant improvement on the calculation of RH. The ratios presented in Table 5.1 are used in Section 7.2.2 to estimate the uncertainty on ESP-r stand-alone results and on BES-BEHAM two-way loose coupling results.

![Variation of relative humidity (two days period)](image)

**Figure 5.25.** Variation of relative humidity (two days period)

<table>
<thead>
<tr>
<th>Predictions</th>
<th>Measurements</th>
<th>Two-way loose coupling</th>
<th>Two-way loose coupling</th>
<th>ESP-r Stand-alone</th>
<th>ESP-r Stand-alone</th>
</tr>
</thead>
</table>

**Table 5.1.** Average ratio between measured RH amplitude in the experiment (m) and results by ESP-r stand-alone (P) and two-way loose coupling (p)

<table>
<thead>
<tr>
<th></th>
<th>m/P or m/p</th>
</tr>
</thead>
<tbody>
<tr>
<td>ESP-r Stand-alone</td>
<td>0.62</td>
</tr>
<tr>
<td>Two-way loose coupling</td>
<td>0.11</td>
</tr>
</tbody>
</table>
Figure 5.26 shows the variation of heating energy consumption during a period of 17 days. In general terms, the two-way loose coupling can predict the overall trends in energy consumption. However, two elements jeopardize the comparison between measurements and simulations. Firstly, the problem description assumed that the experimental room was thermally decoupled from the corridor shown in Figure 5.22, hence no information was provided about the temperature in the corridor, or about the materials used in its envelope. The results in Figure 5.26 show the strong dependence between the conditions assumed in the corridor and the energy consumption in the experimental room. The variation in the results depending on the conditions in the corridor is consistent with differences in the solutions reported by different participants of the IEA-ECBCS Annex 41 (Woloszyn and Rode 2008). The level of interaction between the experimental room and the corridor could be inferred from the U-values of the external walls in the experimental room (~0.4 W/K.m²) in comparison with the internal partition between the experimental room and the corridor (~0.6 W/K.m²). Considering the higher thermal transmittance and the large area of the internal partition, it is natural that the corridor plays a role in the energy consumption of the room. A second element that compromises the comparison is the apparent noise in the energy consumption, which is not consistent with the experimental setup and is consequently not visible in the simulation results. There are no direct solar gains, no variations in the internal heating gains, no variations in the infiltration rate, no sudden

![Figure 5.26. Variation of heating energy consumption (17 days period)](image-url)
variations in the external temperatures or in any other feature that could justify the noise observed in the measurements. In some cases, the noise is responsible for readings above 1000 W, which is the nominal maximum power of the heater used in the experiments (Woloszyn and Rode 2008). Therefore, the noise in the measurements should not be taken into account in the comparison. Considering these elements, the agreement between the two-way loose coupling and the measurements is quite good, and thus the prototype was validated for heating energy consumption calculations.

5.7 Validation and limitations of coupling protocols A and B

5.7.1 Problem outline

In the previous five sections, the prototype developed using two-way loose coupling was validated. This prototype results from the implementation of the coupling protocol C, the most comprehensive of the three described in Section 3.10. Coupling protocols A and B are both based on one-way coupling, and therefore they cannot capture any feedback between the building envelope and the interior domain. However, one-way coupling is routinely used in order to provide boundary conditions for stand-alone BEHAM applications. Hence, this section addresses the validation of the coupling protocol A (one-way coupling using indoor air states) and the prototype program based on coupling protocol B (one-way coupling using flux equation). Results obtained with the validated two-way loose coupling prototype were used as reference data in this validation exercise. The BESTEST case 600 building is used in this exercise, as described in the IEA-ECBCS Annex 41 and summarized in Figure 5.14 (Woloszyn and Rode 2008). For clarity, the analysis is focused only on the west wall.

Both coupling protocols A and B are focused on the provision of data for the interior boundary conditions in BEHAM programs, and therefore the focus of this section should remain on the interior boundary condition. Usually, BEHAM programs have models to calculate the exterior boundary condition, and HAMFEM is not an exception. However, the calculation of exterior boundary conditions by HAMFEM differs from ESP-r and it might lead to differences in the results that are not relevant for this validation exercise. In order to provide a fair comparison between the coupling protocols, the values for the exterior boundary condition in HAMFEM were extracted from calculation using the two-way loose coupling prototype. This procedure assured that the exterior boundary condition was identical in all simulations performed in this section and any discrepancies in the results can be attributed to the focus of this section, i.e. the coupling protocol used to calculate the interior boundary condition.
5.7.2 Coupling protocol A – results and discussion

In the coupling protocol A (one-way coupling using indoor air states), ESP-r stand-alone was used to calculate the interior air temperature and RH, which will be later used as boundary conditions by HAMFEM. Figure 5.27 compares the results of interior surface temperature obtained using the validated two-way loose coupling prototype with the results obtained by one-way coupling using indoor air states. From the figure it is clear that one-way coupling using indoor air states underestimates the interior surface temperature, in this particular case with differences up to 16 °C. One-way coupling also overestimates the temperature in a few hours during summer, up to 5 °C. These large deviations can be attributed to assumptions used in BEHAM to define interior boundary conditions, based solely on indoor air states. The first assumption is the validity of combining convection and LW radiation in a single coefficient, i.e. air temperature is approximately equal to the surrounding surface temperatures. Figure 5.28 shows that in the case of this particular building, this assumption is not valid. Although the BESTEST building is atypical, the validity of this assumption is compromised in rooms with large windows, due to the temperature differences between walls and glazing, but mainly due to the incoming SW radiation in the room. This is connected to the second assumption in the use of indoor air states as boundary conditions in BEHAM: the absence of direct SW radiation. Figure 5.29 shows that this assumption is also not valid for this building and location, and that SW radiation plays a major role in the heat flux at the interior surface under analysis.

![Figure 5.27. Temperature at the interior surface using coupling protocol A](image-url)
5. Validation

![Figure 5.28. Air temperature and MRT - BESTEST case 600 building](image)

![Figure 5.29. Heat fluxes at the internal surface - BESTEST case 600 building](image)

From the above, it can be concluded that one-way coupling using indoor air states is valid only under very particular circumstances. Therefore, it should only be used when the validity of these assumptions can be verified. Possible applications of coupling procedure A could be for buildings with small windows, good glazing and located in high latitudes and evaluated for winter conditions.

5.7.3 Coupling protocol B – results and discussion

In the coupling protocol B (one-way coupling using flux equations), ESP-r stand-alone is used to calculate the equations of heat and moisture fluxes as a functions of the surface states, which will be later used as boundary conditions by HAMFEM. Figure 5.30 (A) shows that for this particular building and location, one-way coupling using flux equations provides very good agreement with results of temperature obtained using two-way loose coupling (differences up to 1.4 °C). This difference is very small when compared to the differences shown in Figure 5.27. Although promising, this good agreement is particular to heat transfer, because ESP-r stand-alone has a detailed heat transfer engine. This is not the case for moisture transfer calculation, and, as indicated
in Figure 5.30 (B), differences of up to 24% in the RH humidity of the interior surface can be observed in the results. These discrepancies can be attributed to the dominant effect of moisture buffering in this particular problem, which cannot be evaluated using ESP-r stand-alone. In cases where the moisture content in the interior air is dominated by other factors, such as high ventilation rates or HVAC systems with humidity control, one-way coupling using flux equations can provide a less expensive alternative to two-way coupling. Moreover, the use of moisture buffering models, such as the effective moisture penetration depth (Kerestecioglu et al. 1990), could potentially improve ESP-r stand-alone calculation, extending the applicability of one-way coupling using flux equations.

![Figure 5.30](image)

**Figure 5.30**. Difference between states at the interior surface calculated using one-way coupling with flux equations and two-way coupling

### 5.8 Conclusions

The validation presented in this chapter allows the following conclusions to be made:

- The prototype program using two-way loose coupling (coupling protocol C) is validated analytically, by inter-model comparison and by comparison with experimental results.
- Two-way loose coupling of BES and BEHAM provides results as accurate or more accurate than stand-alone BES or BEHAM simulations.
- The use of CFD-HAM provides a valuable step between isothermal moisture transfer analytical solutions and more realistic problems used in validation of whole-building HAM simulations.
- The problem of combined heat and moisture transfer in the solid and fluid domain with a step change in the boundary conditions has a high sensitivity
to convective transfer coefficients, highlighting the importance of coupling with CFD to determine these coefficients in whole-building HAM simulations.

- The apparent large dispersion of results found in some inter-model comparisons carried out during the IEA-ECBCS Annex 41, such as the simplified BESTEST building and the BESTEST case 600, can be mainly attributed to outlier results. Discarding these outliers demonstrated that most solutions are in good agreement, and therefore provide a valuable result for whole-building HAM validation.

- In the cases evaluated, moisture transfer does not play a major role in the following PIs: energy demand, peak power demand, interior air temperature, temperatures within building elements.

- Moisture transfer plays a major role in the calculation of interior air RH. The ratio between the daily amplitude found in the measurements and the amplitude according to stand-alone BES predictions is 0.62.

- Initialization of moisture content of walls plays a major role in the BESTEST case 600 inter-model comparison carried out during IEA-ECBCS Annex 41. Different initializations can, to a large extent, explain the variation in the solutions proposed for this exercise.

- One-way coupling using indoor air states (coupling protocol A) has a limited applicability due to assumptions used in this type of boundary condition, and therefore its use should be avoided unless the validity of such assumptions can be verified for the case under evaluation.

- One-way coupling using flux equations (coupling protocols B) is a reliable and less expensive alternative to two-way coupling in cases where the interior air RH is not dominated by moisture buffering effects.
6

Coupling necessity decision procedure

6.1 Introduction

CBPS programs cover a very large range of applications, for different building typologies, geometries, climates, etc. These programs are used to predict several PIs, and for each specific case, the minimum required accuracy is different. Accuracy requirements depend on economical, technological and social constraints from designers, contractors and final users.

In order to meet accuracy requirements, CBPS can be performed at different levels of complexity and resolution, leading to different uncertainties in the calculation. In the case of PIs for HAM engineering, calculations can be performed using methods as simple as steady-state calculations, such as the Glaser method, or as complex as the two-way coupled simulation developed in the present research.

As demonstrated in the previous chapter, two-way coupled BES-BEHAM simulations can reduce the uncertainty in the prediction of some PIs for buildings. However, in several cases stand-alone BES or BEHAM programs can provide results sufficiently accurate for the intended use, even considering their uncertainties. In these cases, the use of coupled BES-BEHAM simulations is not justified and should be avoided.

This chapter describes a procedure developed in this thesis to evaluate the necessity of using BES-BEHAM coupled simulations to address a particular problem. This procedure, named Coupling Necessity Decision Procedure (CNDP), indicates the actions necessary to define the correct modelling resolution for a specific building and PI. The overall concept used in the CNDP is presented in Section 6.3, followed by a discussion about the role of uncertainty and sensitivity analysis in the CNDP. In the last part of this chapter, two specific CNDPs are proposed, for PIs related to the indoor environment or to building elements.
6. Coupling necessity decision procedure

6.2 Qualitative assessment of simulation applicability

The first chapter of this thesis describes several arguments in favour of CBPS. However, in some cases CBPS may not be the best way to address a problem. Hence, before describing the decision method to assess the applicability of coupled BES-BEHAM simulations, it is useful to recall some cases where the use of any CPBS is not recommended.

Firstly, CBPS costs time, and requires highly trained personnel and sophisticated software and hardware. In cases where these resources are not available, the use of CBPS should be avoided, otherwise it may compromise the results obtained (Banks and Gibson 1997).

Secondly, CBPS should not be used to solve problems for which the solution is already known. There is a huge body of knowledge about building pathologies, their causes and known remedies. In these cases, mistakes made by others in the past could save time and resources by removing the need for unnecessary CBPS studies (Banks and Gibson 1997).

Thirdly, one should keep in mind that standard CBPS often do not take into account problems related to bad workmanship, which are the bases of several moisture pathology problems. CBPS usually assumes that construction is carried out in accordance to the design and best practices. If this is not the case, results of CBPS will predict a performance much better than the one found in the real building.

In the light of these arguments, one might argue that the applicability of CBPS is very limited. However, this is not the case. Every day, designers are evaluating innovative solutions aiming at the improvement of building performance, reduction of costs, gains in productivity, etc. In most cases, the performance of such solutions is not known and CBPS can provided detailed information to help responsible designers in making the numerous decisions involved in the construction or renovation of a building.

Last but not least, coupled BES-BEHAM simulations necessarily require expertise in BES stand-alone and BEHAM stand-alone, in order to follow best practice guidelines when using both programs. Users without this expertise should not use coupled BES-BEHAM simulations.

6.3 General CNDP

The definition of CNDP has been addressed in the past for coupled simulations between BES and CFD (Djunaedy et al. 2004, Djunaedy 2005, Mirsadeghi et al. 2010).
Using the concepts presented in this previous research, a general purpose CNDP was developed in this thesis and is presented in Figure 6.1. The CNDP has four inputs: physical process, building, PI and target value. The inputs are very important because they indicate that outcomes of CNDP are case dependant in these four aspects, as described in the next paragraphs.

The CNDP described in Figure 6.1 can be applied to any case of coupled simulations; however the need for coupled simulations depends on the physical phenomenon addressed in the coupled simulation. In this chapter, the objective is to define the need for BES-BEHAM coupled simulations, therefore the HAM transfer is the physical process under analysis.

![Figure 6.1. General CNDP](image)

The building’s characteristics, use and location play an important role in CNDP. For example, a building with a water-proof envelope, such as a fully glazed building, might be accurately simulated using stand-alone BES, while a historic building with a hygroscopic envelope might need coupled BES-BEHAM simulations.

Previous knowledge about the PI to be obtained with the simulation is also important to define the correct modelling resolution. For example, stand-alone BES might be adequate to calculate the energy demand of an office building, but it might not be accurate enough to assess mould growth risk, which could demand coupled simulations.

The evaluation of building performance is usually carried out to design buildings that respect certain target values for each PI. These target values are defined by the designer, by legislation, by codes for sustainable building, etc. Considering the need to
meet a target value, the simulation does not need to provide exact results, but it must provide results accurate enough to allow designer to judge if the building is below or above the target value.

The results of the general CNDP are exemplified for three buildings (A, B and C) in Figure 6.2, where the CNDP is used to evaluate the need for coupled BES-BEHAM simulations (physical process) to calculate the cooling energy demand (PI). Building A, for example, has a maximum allowed cooling energy demand of 7.1 MWh (target value), and the deterministic result of BES stand-alone simulation is 6.7 MWh (gray bar). Based only on this deterministic result, it could be concluded that Building A respects the maximum allowed cooling energy demand. However, the BES stand-alone simulations adopt several assumptions and simplifications that might lead to errors in the results. In Figure 6.2, these possible errors are indicated by uncertainty bars, which show that the actual cooling energy demand is some value between 4.8 to 8.6 MWh. In this case, the simulation is inconclusive, because it is not possible to assess if Building A meets the target value or not. Therefore, Building A demands a simulation with lower uncertainty, which can be obtained using, among other means, an improved modelling resolution, such as coupled BES-BEHAM simulations.

Results for Building B have smaller uncertainty when compared to Building A, and in this case the results are conclusive because all values in the uncertainty range indicate that Building B is above the target value. There is no doubt that the design of Building B does not meet the requirements of maximum energy demand, hence, there is no need to use an improved modelling resolution and the result of BES stand-alone simulation can be accepted. The same applies for Building C, where it is clear that the cooling energy demand is below the target value in spite of the large uncertainty in the results, i.e. this design certainly meets the requirements of maximum energy demand.

**Figure 6.2 . Example of uncertain results compared to target values for a PI**
The general CNDP demonstrates the important role played by uncertainty of CBPS results in the selection of appropriate modelling resolution to address a given design problem. However, most CBPS programs do not provide the uncertainty associated with the mean deterministic results. The next section addresses the different sources of uncertainty in CBPS.

### 6.3.1 Uncertainty analysis

This thesis adopts a definition of uncertainty in CBPS derived from the uncertainty in metrology (ISO 1998). Here, uncertainty in CBPS is defined as a parameter, associated with the deterministic result of a CBPS program that characterizes the dispersion of the values that could reasonably be attributed to the real quantity being modelled by the program. This definition provides flexibility to the uncertainty analysis because it is focused not on specific sources of uncertainty, but rather on the overall impact on the results of calculations.

Uncertainty analysis in CBPS has been studied for several years (de Wit 2001, Macdonald and Strachan 2001, Macdonald 2002, Macdonald and Clarke 2007, Struck and Hensen 2007, Hopfe 2009, Struck et al. 2009). These studies address only one source of uncertainty: the simulation input. Inputs are indeed a major source of uncertainty in CBPS, because CBPS programs might have a large number of inputs and many of them have large uncertainty. The propagation of uncertainties from inputs to the simulation results can be calculated using, for example, Monte Carlo analysis. Figure 6.3 represents the propagation of input uncertainties (stochastic inputs) in a deterministic model, leading to a probability distribution of results (stochastic output). The focus of CNDP is not on the input uncertainties because all models, as simple as the Glaser method or as complex as BES-BEHAM coupled simulations, might suffer from input uncertainties. However, a simple model cannot provide accurate results even when very accurate inputs are adopted. For example, results obtained using the Glaser method have a large uncertainty, but this uncertainty is not derived from input uncertainties. In this case, the uncertainty is derived from the assumptions and simplifications incorporated in the model. These uncertainties are referred to in this thesis as modelling uncertainties, and the total uncertainty in the results is a combination of input uncertainties and modelling uncertainties. Modelling uncertainties do not depend on stochastic inputs to produce stochastic outputs, as represented in Figure 6.3. Although important, information about modelling uncertainty is rarely available. Most, if not all, CBPS programs do not have any quantification of their modelling uncertainty, i.e. there is no quantitative information about how well results
calculated using a CBPS program agree with experimental data obtained for the whole range of applications of the program. The lack of information on modelling uncertainty is the primary constraint for the use of CNDP, because it is hard to evaluate the benefit of using a higher modelling resolution when the uncertainty in the results using a lower modelling resolution is unknown.

A CNDP designed to assess the need of BES-BEHAM coupling demands information on the input uncertainties and modelling uncertainty in stand-alone BES and BEHAM simulations. This problem is addressed in the following paragraphs.

In stand-alone BEHAM simulations, the main sources of modelling uncertainty related to BES-BEHAM coupling are located in the boundary conditions. Boundary conditions in BEHAM are usually calculated using input parameter described in text files for the interior and exterior domains. It makes the calculation of these sort of modelling uncertainties in BEHAM very straightforward because the text files can be used to emulate the modelling uncertainty using input uncertainties.

In stand-alone BES simulations, the calculation of modelling uncertainty related to BES-BEHAM is more difficult than in BEHAM, because the sources of uncertainty are embedded in the core of the calculation engine. Simplification in the moisture transfer calculation may affect, for example, the:

- Thermal conductivity as a function of the moisture content.
- Thermal capacity as a function of the moisture content.
- Sources/sinks of moisture at the interior domain due to the flux from/to the building envelope and internal partitions.
- Sources/sinks of heat due to latent heat exchange in the building envelope and internal partitions.

Part of these features can be emulated using input uncertainties, but this depends on two factors. Firstly, it is necessary to evaluate the existence of one or more inputs in BES that could be used to emulate a certain effect. The thermal conductivity, for example, is a common input in BES programs, and its input uncertainty can be used...
to emulate the presence or absence of moisture, usually using extreme values (dry/saturate). The same applies to the thermal capacity. Sources/sinks of moisture at the interior domain are also common input values in BES, which can be used to emulate the effects of flux from/to the building envelope and internal partitions. However, there are cases where uncertainty due to latent heat exchange cannot be emulated using this approach, because there is no input to describe sources/sinks of energy in all nodes of the building envelope and internal partitions. The impossibility of emulating latent heat exchange effects in all BES nodes demonstrate the limitations of the use of input uncertainties to evaluate modelling uncertainties.

Secondly, it is necessary to evaluate if the selected input variable is not calculated by the BES program using a simplified model. In some BES programs, the thermal conductivity, for example, can be treated as a fixed input value or it can be calculated based on the moisture content obtained using simplified vapour transfer models. Although these simplified models have deficiencies when compared to BEHAM programs, they provide thermal conductivity values that are more accurate than fixed inputs. In some cases, simplified models could provide results accurate enough for a given use. However, this possibility cannot be properly evaluated using input. Simplified models should be disabled in order to assess the worst case scenario of BES modelling uncertainty, but this will certainty lead to some overestimation in the uncertainty.

One example of the use of input uncertainty to emulate modelling uncertainty is provided by previous research, aiming to evaluate the need of coupled BES-CFD simulations (Djunaedy et al. 2004). In this previous research, the interior convective heat transfer coefficient (hc_i) was selected as the input variable to emulate the uncertainties related to different flow and convection regimes. In many BES programs, hc_i can be provided by users as a fixed input value or it can be calculated by BES using a simplified data-driven model. As described above, the data-driven model had to be disabled. Therefore, the modelling uncertainty in the simplified data-driven model itself is not evaluated, and consequently there is no information about the accuracy in the predictions of this simplified data-driven model.

In this section, the uncertainty in the results is classified according to its source in: input uncertainty and modelling uncertainty. Uncertainty analysis is a valuable technique to evaluate the accuracy of CBPS results. However, it does not indicate the role played by each type of input data in the overall uncertainty. In some cases, CBPS results have a large uncertainty, but the physical process under analysis on the CNDP might not be among the most important sources of uncertainty. In these cases,
improvements in the physical model might not produce a significant reduction in the uncertainty; hence, these improvements should be avoided. This topic is addressed in the next section.

6.3.2 Sensitivity analysis

The focus of CNDP is on the modelling uncertainties related to the specific physical processes addressed in the coupled simulation. In the particular case of coupling between BES and BEHAM, the CNDP is focused on modelling uncertainties related to the combined HAM transfer in the whole-building scale. Sensitivity analysis can be adopted to evaluate the importance of each specific input, or the modelling uncertainties in relation to the overall uncertainty in the results (Hopfe 2009). Figure 6.4 exemplifies the outcomes of a sensitivity analysis carried out using stand-alone BES simulations for a certain PI in the Buildings A and B. The input data with a higher impact on the overall uncertainty can be identified at the top of the figure. In the case of Building A, the specific physical processes addressed in the coupled simulation (dark gray bars) are not among the main sources of uncertainty, therefore a coupled simulation is not recommended. The uncertainty in the results for Building A can be reduced by using, for example, more accurate data for the ventilation/infiltration rate and for the internal heat gains. In the case of Building B, physical processes addressed in the coupled simulation are among the main sources of uncertainty, therefore the use of coupled simulation is recommended. The next section describes two detailed CNDPs that specify the role of uncertainty and sensitivity analysis in the decision of the adequate modelling resolution.

![Figure 6.4. Example of sensitivity analysis](image)

Figure 6.4. Example of sensitivity analysis
6.4 Detailed CNDPs

The previous section proposed the general CNDP, addressing the case dependant aspect of this type of decision procedure and the role played by uncertainty and sensitivity analysis. In this section, this general CNDP is expanded and enhanced in two detailed CNDPs, addressing the particularities of BES-BEHAM coupled simulations.

6.4.1 Modelling resolution as a function of the PI

The CNDP defines the proper modelling resolution for a given building, PI, target value and physical process. For each PI, there is a primary modelling resolution, i.e. the most straightforward resolution to evaluate the PI. For example, whole-building energy demand is usually evaluated using stand-alone BES simulations, while condensation risk is usually evaluated using stand-alone BEHAM simulations. The existence of different primary modelling resolutions according to the PI shows the need for detailed CNDPs for different PIs.

The definition of the primary modelling resolution for a given PI is the first step to define detailed CNDPs. Table 6.1 describes the suggested primary modelling resolution for some PIs usually evaluated using BES and/or BEHAM programs. In this table, PIs are classified according to their main geometrical domain. This classification is based on: (1) the point(s) in space where the PI is evaluated and (2) capabilities and deficiencies of BES and BEHAM programs (summarized in Table 3.1). In all cases, stand-alone simulations are the primary modelling resolution and two-way loose coupling of BES-BEHAM is the most accurate modelling resolution addressed in this thesis. The hierarchy in the accuracy of these approaches is demonstrated in Chapter 5. Chapter 5 also demonstrated that one-way BES-BEHAM coupling is more accurate than stand-alone BEHAM simulations, therefore one-way BES-BEHAM coupling is included in Table 6.1.

<table>
<thead>
<tr>
<th>Geometrical domain</th>
<th>Performance indicator</th>
<th>Primary modelling resolution</th>
<th>Secondary modelling resolution</th>
<th>Most accurate modelling resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Interior</td>
<td>Energy demand</td>
<td>BES</td>
<td>One-way BES-BEHAM coupling</td>
<td>Two-way loose coupling of BES-BEHAM</td>
</tr>
<tr>
<td></td>
<td>Peak power demand</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Thermal comfort</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>IAQ</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Building envelope</td>
<td>Condensation risk</td>
<td>BEHAM</td>
<td></td>
<td></td>
</tr>
<tr>
<td>and internal partitions</td>
<td>Frost risk</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Mould growth</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Based on Table 6.1, it is possible to construct two detailed CNDPs, according to the PI of interest. These detailed CNDPs are described in the next sections.
6. Coupling necessity decision procedure

6.4.2 Detailed CNDP for PIs in the interior domain

Figure 6.5 represents the detailed CNDP proposed for PIs in the interior domain. Firstly, the CNDP evaluates the PI of interest. Secondly, uncertainty analysis is carried out, using input uncertainties to emulate part of the modelling uncertainty related to simplifications in the moisture transfer in BES simulations. Other sources of uncertainty are also included in the analysis if necessary. Thirdly, results of the uncertainty analysis are compared with the target value, as exemplified in Figure 6.2. If the result is valid, i.e. uncertainty in the results does not compromise the evaluation of the design under study, the model is accepted and the CNDP is concluded. If the results are not valid, sensitivity analysis is carried out to determine the role of each source of uncertainty, as exemplified in Figure 6.4. Sensitivity analysis is only required for the cases where multiple sources of uncertainty are taken into account. Two-way loose coupling of BES-BEHAM should be used when the simplifications in moisture transfer in BES are one of the main sources of uncertainty (exemplified in Figure 6.4 – Building B). Otherwise, it is recommended to reduce the uncertainty originated in other sources of uncertainty (exemplified in Figure 6.4 – Building A).

Figure 6.5 . Detailed CNDP for PIs in the interior domain

As describe in Section 6.3.1, the use of the input uncertainties to emulate part of the modelling uncertainty has severe limitations. In this detailed CNDP, values of thermal conductivity and thermal capacity are used for this purpose, adopting fixed
values (dry/saturate) for each building material over the whole year. In addition, sources/sinks of moisture in the interior air node are used to emulate moisture fluxes between air and building elements. Latent heat is not considered in this detailed CNDP. The use of this detailed CNDP is exemplified in Section 7.3.

6.4.3 Detailed CNDP for PIs in the building envelope

Figure 6.6 represents the detailed CNDP proposed for PIs in the building envelope and internal partitions. As in Figure 6.5, this CNDP first evaluates the PI of interest. Second, uncertainty analysis is carried out in stand-alone BEHAM simulations, using the uncertainty in boundary condition input values to emulate the simplification in the interior and exterior domain. Results are then compared with the target value, and one-way coupling of BES-BEHAM using flux equations is adopted in cases where results are not valid enough. From this point on, this detailed CNDP is very similar to Figure 6.5.

![Figure 6.6. Detailed CNDP for PIs in the building envelope and internal partitions domain](image)
This detailed CNDP uses input uncertainties to emulate the modelling uncertainty; hence the limitations described in the previous section also apply to this detailed CNDP. In addition, SW radiation might play an important role in the boundary conditions in the interior surface of building elements, as indicated in Chapter 5. However, SW radiation is not an input value in most BEHAM programs. Nevertheless, heat fluxes due to SW radiation can be emulated using high values of interior air temperature.

6.5 Conclusions

This chapter proposes decision procedures to assess the most adequate modelling resolution to simulate a given problem. It also proposes detailed decision procedures applicable for coupled BES-BEHAM simulations. The content of this chapter allows the following conclusions to be made:

- The definition of most adequate approaches for simulations is a case dependant problem, also depending on the performance indicator expected as a result of the simulation.

- Building characteristics, location and use are relevant input data in the decision procedure.

- The use of target values of performance indicators allows the assessment of the validity of a modelling resolution to simulate a particular design, indicating if the uncertainty in the results does not compromise the evaluation of the design under study.

- Uncertainty and sensitivity analysis provide valuable information for the definition of most adequate modelling resolution.

- Lack of information about the modelling uncertainty can, in some cases, be overcome by emulating modelling uncertainty using input uncertainty.

- The classification of performance indicators according to their location in space (interior and building envelope/internal partitions) allows the construction of detailed CNDPs, based on different primary modelling resolutions (stand-alone BES and stand-alone BEHAM simulations).
7

Applications

7.1 Introduction

The main objective of this research was to develop ways and means to couple BES and BEHAM programs, and the last chapters described in detail the four deliverables listed in Section 1.4, i.e. coupling protocols, prototype software, coupling validation and the CNDP. This chapter provides two examples of applications in order to illustrate the potential uses of the prototype software and the CNDP. However, these examples only address a small portion of the range of possible uses for the knowledge and tools developed in this thesis, which is certainly much broader in reality. Section 7.2 describes the use of CNDP to assess mould growth risk in the BESTEST case 600 building. In the assessment of mould growth risk, several modelling resolutions are applied demonstrating that two-way loose coupling is actually necessary to assess this PI in this particular building. Section 7.2 provides an example of the use of CNDP to evaluate the need for BES-BEHAM coupled simulations for the calculation of annual energy demand of a terrace house in the Netherlands. In the calculation of annual energy demand for this particular building, the CNDP demonstrates that stand-alone BES simulation provides accurate results, hence BES-BEHAM coupled simulations are not necessary.

7.2 Mould growth risk assessment

7.2.1 Problem outline

The presence of mould in the indoor environment is associated with asthma, which “is a leading chronic disease among children and poses a significant burden on public health” (Jones et al. 2010). This application example addresses the assessment of mould growth risk in the BESTEST case 600 building (Figure 5.14), as described in the IEA-ECBCS Annex 41 (Woloszyn and Rode 2008). Most mould growth risk assessment methods rely on CBPS to provide data about the surface states (temperature and RH) over time (Sedlbauer 2001, Krus and Sedbauer 2005, Moon
These states are then compared with curves that describe the germination and/or the growth rate of mould under certain conditions of temperature and RH, such as the mould germination graphs by Smith and Hill (1982) or by Sedlbauer (2001). The graph by Smith and Hill (1982) for *Aspergillus restrictus* is adopted in this exercise, due to its good trade-off between accuracy and simplicity (Moon 2005).

Figure 6.6 describes the CNDP for PIs in the building envelope and internal partitions domain, which is the case of mould growth risk. This CNDP indicates the successive use of three modelling resolutions: one-way coupling using indoor air states (which is in fact very similar to stand-alone BEHAM), one-way loose coupling using flux equation and finally two-way loose coupling. In addition to these modelling resolutions, ESP-r stand-alone simulations are performed because it is common practice to use stand-alone BES simulation to predict mould growth. In this case, the surface humidity ratio is assumed to be equal to the air humidity ratio.

### 7.2.2 Quantification of modelling uncertainty

Quantifying modelling uncertainty is fundamental to assess the validity of different modelling resolutions using the CNDPs proposed in Chapter 6. The main source of uncertainty in this case study is the moisture buffering in the zone, which modifies the RH in the interior air node and in the interior surface node. As described in Section 6.3.1, information about modelling uncertainty is rarely available. In the present case, the modelling uncertainty should indicate how accurate the stand-alone ESP-r results are, bearing in mind the fact that it does not take into account moisture transfer and accumulation. Modelling uncertainty of the two-way loose coupling prototype should preferably be available as well. Two-way loose coupling is more accurate than other modelling resolutions. However, as any other model, two-way loose coupling is not a perfect description of reality, presenting also some degree of modelling uncertainty. Information on modelling uncertainty can be obtained by the systematic comparison of experimental results and simulation results, which should necessarily consider experiments with similar characteristics and scope of the intended simulation. This section uses the comparison of experimental results and simulation described on Section 5.6.2 to estimate the modelling uncertainty in ESP-r stand-alone and in the two-way loose coupling results.

The use of the results from Section 5.6.2 to quantify modelling uncertainty is not advisable for every case, because the uncertainty in RH results depends on several factors, such as air change rate, amount of hygroscopic material exposed in the internal
domain, moisture permeability and capacity of materials, moisture load in the internal and external domains and the use of vapour barriers. The use of the results from Section 5.6.2 is possible here due to similarities between this case study and the building used in Section 5.6.2. In both cases the interior finishing is the same, as well as the ventilation rate. Moreover, the amount of hygroscopic material exposed is similar, as is the hygroscopic load in the interior domain. In an ideal scenario, the modelling uncertainty for this particular case would be quantified based on comparisons of simulation results and experiments for a large range of cases. This comparison would lead to statistical models that would describe the uncertainty as function of factors which influence this uncertainty, listed in the beginning of this paragraph. This type of statistical model is currently not available and its development is out of the scope of this thesis. However, results of Section 5.6.2 provide a first approximation of the modelling uncertainty in stand-alone ESP-r results and in two-way loose coupling results in line with the purpose of this section. Paragraphs below describe the methodology adopted to derive the modelling uncertainty related to moisture transfer using the simulation results and the results of Section 5.6.2. Other sources of uncertainty are not taken into account in this case study.

Results presented in Table 5.1 (Section 5.6.2) provide a comparison between simulations and experimental results, allowing some degree of evaluation of the modelling uncertainty in the results. Using this table and ESP-r stand-alone results, it is construct a curve that possibly describes the daily RH variation, showing the reduced amplitude observed in the experiments. This curve is presented in Figure 7.1, and it is adopted as the uncertainty limit for this particular problem. This uncertainty limit curve is used in the mould growth analysis in this section. It is assumed that the area in Figure 7.1 which is between ESP-r stand-alone results and the uncertainty limit curve represents the uncertainty range of the simulation.

The next section shows the results obtained with different modelling resolutions plotted over the germination graph proposed by Smith and Hill (1982). Some methods to analyse mould growth are based on the amount of consecutive hours in which germination might occur (Moon 2005). However, in the present case study the occurrence of consecutive hours is not taken into account and the focus is kept on the use of CNDP and the different prototypes developed in this thesis.
7. Applications

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Figure 7.1. Uncertainty in ESP-r stand-alone predictions of RH, calculated based on results from Section 5.6.2 (Table 5.1)

7.2.3 Results and discussion

Figure 7.2 shows results obtained with the lowest modelling resolution adopted in this case study, i.e. BES stand-alone. Germination is expected to occur in the area defined by isopleths on the top of the graph. In Figure 7.2, the uncertainty limit simulation results are presented and they indicate the risk of mould growth during some hours and maximum RH near to 90%. Figure 7.2 shows also the uncertainty limits as discussed in the previous section. In the scenario represented by the uncertainty limit, there is no risk of mould growth. Consequently, it is clear that ESP-r stand-alone simulation is not valid and an enhanced modelling resolution regarding modelling of moisture should be used. For this case study, sensitivity analysis was not performed because only sources of uncertainty related to simplification in modelling of moisture were taken into account.

Figure 7.3 shows results obtained using one-way coupling using indoor air states, where the same pattern as in Figure 7.2 can be observed. Deficiencies of this coupling procedure regarding SW and LW radiation are not clearly shown in these graphs, because the maximum surface temperatures are in the same order of magnitude of ESP-r stand-alone (only 5 °C of difference). However, surface temperature predicted using one-way coupling using indoor air states are in general lower than ESP-r stand-alone for most hours in the year, which can be better observed at low RH levels in Figure 7.3. The uncertainty in RH results of ESP-r stand-alone is reflected in the results of one-way coupling, leading to maximum RH of 90% and risk of mould growth according to the simulation results. However, the uncertainty limit
shows a scenario where there is no risk of mould growth. Consequently, the simulation is not valid and thus a higher modelling resolution should be applied.

**Figure 7.2.** Mould growth risk assessment obtained using BES stand-alone

**Figure 7.3.** Mould growth risk assessment obtained using one-way coupling using indoor air states
Figure 7.4 shows the results obtained using one-way coupling using flux equations, which provide a considerable reduction in the uncertainty when compared to Figure 7.2 and Figure 7.3. Reduction in the maximum surface RH, from 90% to 80%, is associated with an increase in the surface temperature due to SW and LW radiation (not considered in Figure 7.2) in combination with coupled heat and moisture transfer (not considered in Figure 7.3). These results confirm the finding of Section 5.7.3 about the improvements related to the use of flux equations. Results also indicate that there is a small risk of mould growth for this particular building. The actual existence of this risk can be assessed using two-way loose coupling, which can greatly reduce the modelling uncertainty in the results when compared to one-way coupling using flux equations, as demonstrated in Chapter 5.

Figure 7.4. Mould growth risk assessment obtained using one-way coupling using flux equations

Figure 7.5 shows results obtained using the validated two-way loose coupling prototype. Simulation results are shown in Figure 7.5(A) and the uncertainty limit calculated using results from Table 5.1 is presented in Figure 7.5(B). The uncertainty in this modelling resolution is much lower, and Figure 7.5 indicates that maximum RH in both simulations are very similar. The maximum RH is actually much lower than the predictions obtained using lower modelling resolutions, indicating that moisture buffering plays a major role in the results. Results in Figure 7.5 are in the uncertainty range described in the previous figures of this section, indicating that the uncertainty
was correctly estimated. Results in Figure 7.5 also show the usefulness of CNDP, demonstrating that for this particular case two-way loose coupling is actually necessary to obtain valid predictions for this PI.

Based on the results obtained using the validated two-way loose coupling prototype, it is possible to evaluate the magnitude of errors that might occur when using lower modelling resolutions for this particular problem. Stand-alone BES and one-way coupling using internal air states overestimate the maximum RH, predicting values around 90 % RH when compared to a more reliable estimate obtained by two-way loose coupling, which indicates maximum around only 65 % RH. Maximum RH calculated by one-way coupling using flux equations is 80 % RH, which represents a significant improvement of accuracy with this modelling resolution.

![Simulation results (A) and Uncertainty limit (B)](image)

Figure 7.5. Mould growth risk assessment obtained using two-way loose coupling

### 7.3 Energy demand in a heavy-weight house

#### 7.3.1 Problem outline

This application example addresses the calculation of annual heating energy demand of an end terrace house in the Netherlands, illustrated in Figure 7.6. The house has a large cavity wall (non-retrofitted) exposed to the exterior environment. Energy demand is not usually sensitive to moisture transfer and accumulation on walls, as demonstrated in Sections 5.4 and 5.5. However, the role of moisture in the energy consumption calculation is case dependant and the CNDP can help to identify cases
where moisture might play a significant role. The CNDP in Figure 6.5 is used, and the sources of uncertainty related to moisture transfer are emulated by changing the thermal conductivity and thermal capacity according to three moisture content values; dry, 99 % RH and saturated. In order to simplify the analysis, other sources of uncertainty are not included in this exercise. The BES program IES-VE is adopted, demonstrating that the decision procedure is not program dependant.

![Terrace house used in the case study](image)

**Figure 7.6 . Terrace house used in the case study**

### 7.3.2 Results and discussion

Figure 7.7 shows results obtained in three simulations using material properties relative to different moisture contents in the outer leaf of the cavity wall. Results clearly indicate that moisture plays a minor role in the energy consumption of this house. In all three simulations, results are much higher than the target value for this PI, indicating the need to renovate the building in order to bring it to current standards.

![Variation in energy demand due the moisture content of walls](image)

**Figure 7.7 . Variation in energy demand due the moisture content of walls**
7.4 Conclusions

This chapter presented two examples of applications that illustrate the potential uses of the prototype software and the CNDP developed in this thesis. Based on these applications, the following conclusions can be made:

- Both detailed CNDPs developed in Chapter 6 proved to be useful in the decision making of the adequate modelling resolution to address realistic problems.

- For the mould growth risk assessment, lower modelling resolution such as BES stand-alone and one-way coupling using indoor air states show large disagreement with results obtained using the validated two-way loose coupling prototype, indicating that these lower modelling resolutions are not valid to study this PI in this particular building.

- For the mould growth risk assessment, one-way coupling using flux equations provides significant improvements in relation to one-way loose coupling using indoor air states. However, uncertainty in the calculation of RH in BES, due to moisture buffering for example, compromises the results of one-way coupling using flux equation.

- Two-way loose coupling of BES-BEHAM was successfully adopted to perform mould growth risk assessment in a realistic case.

- For the case of a terrace house in the Netherlands, the heating energy demand is not sensitive to moisture accumulation on walls, confirming similar results from Chapter 5.
Conclusions

8.1 Concluding remarks

This thesis hypothesizes that coupled simulation of building energy simulation (BES) and building element heat, air and moisture transfer (BEHAM) programs can provide equally accurate or more accurate results for whole-building HAM simulation than stand-alone BES and BEHAM applications. The evidence presented in this thesis, particularly in Chapters 5 and 7, cannot be used to prove that this hypothesis is false. In fact, the results demonstrate the validity of this hypothesis under a range of tests. Therefore, the primary conclusion of this thesis is that, until new evidence is presented, the coupling of BES and BEHAM does indeed improve the overall accuracy of whole-building HAM simulation when compared to stand-alone simulations. In the previous sentence, the term “overall” indicates that in some cases there is a significant improvement, particularly in the calculation of relative humidity (RH), while in other cases results from coupled simulations are as good as those from stand-alone simulations. In order to distinguish the cases where coupling can in fact improve the accuracy of the results, the coupling necessity decision procedure (CNDP) was formulated in Chapter 6 and was successfully applied in Chapter 7. The CNDP provides practitioners with a valuable tool to define the appropriate modelling resolution for realistic projects.

This thesis provides a number of secondary results, which are summarized at the end of each chapter. Chapter 2 provides an overview of projects dealing with BES and BEHAM integration, clarifying the innovativeness of the approach used in this thesis. In Chapter 3, the concept of coupling procedure is introduced, which facilitates on a large scale the development of coupled simulations. Chapter 3 also describes the use of TCP/IP sockets for inter-process communication, which opens new frontiers in the development of coupled simulations by different developers working in different institutions and performing coupled simulation via the internet. Chapter 4 presents a detailed description of the modifications carried out in ESP-r and HAMFEM. Chapter 4
also pays close attention to verification, which is usually disregarded in academic software development. The mechanisms and exercises used in the verification described in Chapter 4 provide a thorough verification, which can, with small modification, be applied in any development of coupled simulations.

Another important secondary result of this thesis is the evaluation of inter-model comparisons carried out in the framework of the Annex 41 of the Energy Conservation in Buildings and Community Systems (ECBCS) Programme, of the International Energy Agency (IEA). IEA-ECBCS Annex 41 results showed very large discrepancies in the solutions provided by different institutions for problems of relative simplicity, usually problems addressing a single zone with only a few uncertainties. Using the validated prototype computer program developed in this research, it was possible to identify a few parameters that have a large influence in the result. Detailed information about these parameters, such as the initialization of moisture content in the wall, was not included in some exercises, leading to a range of solutions in apparent disagreement. Results from Chapter 5 demonstrate that the whole-building HAM simulation community has the potential to obtain consensus on the solution of simplified problems, leading to benchmark solutions that can be used as part of the validation of new software.

8.2 Directions for future work

In face of the findings of this thesis, a number of directions for future work can be foreseen.

The first and possibly the most relevant one is the quantification of modelling uncertainties in different modelling resolutions. The validation presented in Chapter 5 demonstrates that BES-BEHAM coupling reduces the modelling uncertainty when compared to stand-alone simulations. However, this thesis does not quantify this improvement on a statistical basis, considering a large range of cases where whole-building HAM simulation can be applied, i.e. different climates, building types and PI.

Results of Sections 5.4 and 5.5 indicated that a few sources of uncertainty partially compromised some of the inter-model comparison carried out during IEA-ECBCS Annex 41. These results indicate the need for further inter-model comparison exercises of whole-building HAM simulation, particularly in cases where liquid load is used as boundary condition, which were not addressed in IEA-ECBCS Annex 41. It is also advisable that further inter-model comparison exercises are carried out in at least two rounds of simulations to allow the participants to evaluate the discrepancies between their models.
The results of Sections 5.3 and 5.5 demonstrated the relevance of further studies using sensitivity and uncertainty analysis in whole-building HAM simulation in order to clarify the input data and boundary conditions that actually play a major role in the results. Uncertainty and sensitivity analysis have been used in BES for more than 10 years, but its use to study whole-building HAM simulation is still embryonic, as well as in stand-alone BEHAM simulation.

Results of Section 5.6 indicated the need for enhanced experimental data for the validation of whole-building HAM simulation. Firstly, there is a lack of information about the uncertainty in the measurement results, which compromises the validation process. Secondly, experimental setups are usually oversimplified, neglecting phenomena that can play a major role in the results, such as SW radiation. Thirdly, whole-building HAM simulation is very sensitive to the problem initialization, indicating that full scale experiments under atmospheric boundary conditions must be carried out over long periods to minimize the importance of initial conditions. Fourthly, assumptions regarding boundary conditions should be carefully evaluated because misjudgements in this topic can have a strong influence on the results, as demonstrated in Section 5.6.2.

The results of Section 5.3 indicated the need for the coupling of CFD-BES-BEHAM to perform certain whole-building HAM simulation. The combination of CFD with prototypes developed in this thesis has the potential to improve several aspects of whole-building HAM simulation, such as wind-driven rain calculations, pressure coefficient and convective heat and mass transfer coefficients for both interior and exterior domain. However, due to the large computational resources required by CFD, its use in coupled whole-building yearly simulation is still limited to the research environment. The use of CFD in coupled simulation also requires additional CNDPs in order to avoid its use in cases where lower modelling resolutions can provide valid results.

Chapters 5 and 7 confirmed the importance of moisture buffering for the RH in the interior domain. Coupled BES-BEHAM simulations can be used to study moisture buffering in a variety of situations, and this data can be used to improve simplified moisture buffering models. This process can also be used to estimate the modelling uncertainty in simplified moisture buffering models.

Chapter 4 demonstrated the importance of quality assurance in academic software development, particularly regarding verification. The techniques described in this chapter can be used in the future as part of guidelines for CBPS program development, which are mainly focused on the validation at the present moment.
Moreover, the use of continuous validation of each code version against benchmark results proved to be useful in the development of programs in this thesis. Future work should address the implementation of such procedure for CBPS programs whenever possible.

Chapter 3 introduced the concept of coupling protocols which, in combination with TCP/IP described in Section 3.9, provide the means to develop coupled simulation by two or more developers working remotely and running coupled simulations via the internet. Future work should explore this possibility to evaluate the actual benefits of this form of scientific software development.

Chapter 7 provided two examples of whole-building HAM simulation that can be performed using the prototypes developed in this thesis. The potential of these prototypes is, however, much larger, and future studies can use coupled BES-BEHAM simulation to address a large number of relevant cases. One example is the simulation of surface condensation problems in a number of buildings such as highly insulated buildings (e.g. passive houses), renovation of historical buildings using improved insulation and buildings with radiant cold ceilings. Evaluation of mould growth risk in a variety of buildings can benefit from coupled BES-BEHAM simulations, particularly in medical facilities, schools, elderly housing and other buildings where users are more vulnerable to health problems. Evaporative cooling, both passive and active, can largely benefit from coupled BES-BEHAM, and the importance of low energy cooling strategies will increase if forecasts of global warming come true in the near future. The study of buildings with large amounts of hygroscopic material, such as libraries, paper factories and warehouses, can also be improved using coupled BES-BEHAM simulations. The same applies for historical buildings where most buildings elements are highly hygroscopic and vapour retarders were not available at the time of their construction. Other buildings that can benefit from the results of this thesis are those where detailed control of moisture levels is necessary, such as museums (both exhibition areas and technical reserve). The study of algae and mould growth in facades, which causes deterioration and aesthetic problems, can also be improved using coupled BES-BEHAM simulations. This is only a brief list of particular cases that can be addressed in the future using the outcomes of this thesis.

A number of solutions for each the coupling features described in Chapter 3 were not implemented in any of the prototypes developed in this thesis. Strong coupling is probably the most remarkable one. Although the decision regarding all coupling features is described in Chapter 3 and supported by the literature, future work can
address other alternatives not implemented in this thesis. On the one hand, it can provide new findings, in the case of better performance than the one obtained in this thesis. On the other hand, it can confirm the validity of the decisions taken in this thesis.

This thesis did not focus on the details of coupling regarding air transfer through building elements, which is also not addressed in the validation and application chapters. Future work should evaluate the real possibilities of including air transfer through building elements in whole-buildings HAM simulations. The nature of air transfer through building elements makes the use of simulation very restricted for design purposes regarding this phenomenon. Air transfer is related to cracks and gaps in building elements. The position of this cracks and gaps is not known during the design stage and, in fact, most designs aim to eliminate air transfer. Therefore, air transfer through building elements is seldom used for design purposes when compared to heat and moisture transfer. Nevertheless, simulation of air transfer has a high potential in the research environment, by allowing the evaluation of particular pathologies related to specific types of constructions and climates.

The directions for future work described above are mainly focused on research topics. However, a number of actions described below have the potential to enhance the fast dissemination of findings of this thesis to practitioners.

The results of Section 5.7 demonstrated the advantages of one-way BES-BEHAM coupling using flux equations in comparison to stand-alone BEHAM simulations and one-way BES-BEHAM coupling using interior air states. However, users of stand-alone BEHAM programs might not have the expertise to perform BES simulations. Future work can explore means to facilitate the use of one-way BES-BEHAM coupling using flux equations for users of stand-alone BEHAM programs. One possible alternative, for example, is the use of BES to provide a variety of pre-calculated sets of values for the flux equations, which can be incorporated in stand-alone BEHAM programs.

CNDP is another outcome of this thesis that should be automated to some degree to become useful for general practitioners. The integration of uncertainty and sensitivity analysis into stand-alone BES and BEHAM programs has the potential to lead to a fully automated execution of the CNDP, informing users about the need to use higher modelling resolutions.

The two-way BES-BEHAM coupling prototype developed in this thesis uses parallel computing to perform each BEHAM simulation, however, the code was tailored for servers with several processors available. Future work can improve the code for
parallel computing in personal computers, which are used by most practitioners and researchers of whole-building HAM simulation.

The CBPS programs developed in this thesis are prototypes, i.e. they do not provide a detailed interface and documentation for practitioners. Future work can explore this gap in order to make coupled simulations available for consultancies and graduate students who do not have the time or knowledge to run software written for research purposes.
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Daniel Cóstola was born on the 28th of January, 1977 in São Paulo, Brazil. He studied architecture and urban planning at the University of São Paulo, Brazil. During his studies, he came into contact with computational building performance simulation and the need for integration to assess the performance of the built environment. This experience led to his graduation project, on the development of a user-friendly program for the evaluation of thermal comfort in hot climates. After his graduation, he worked for three years as architect, taking part in complex projects such as the building of the new control centre of São Paulo’s metropolitan rail system, and a social housing development for 8000 inhabitants in Guarulhos, Brazil. In 2006, he returned to the University of São Paulo to conduct MPhil research on predictive methods for natural ventilation simulation. During his MPhil, he received the first prize for the design of the new Brazilian Journal of Post-graduate Studies. This prize allowed him to spend three months working with Prof. David Etheridge at the University of Nottingham, UK, to develop research on wind tunnel modelling of natural ventilation. After his MPhil, Daniel joined the Building Physics and Systems unit at the Department of Architecture, Building and Planning, Eindhoven University of Technology, the Netherlands. During his PhD, he spent 2 months at the Tokyo Polytechnic University, Japan (2009) working with Prof. Masaaki Ohba on the GCOE program.
Publication list

Journal papers


Conference papers


D. Cóstola, B. Blocken, J.L.M. Hensen. 2009. External coupling of BES and HAM programs for whole building simulation. In P.A. Strachan, N.J. Kelly, M. Kummert (Eds.), 11th International Building Performance Simulation Conference, 27-30 July 2009, Glasgow, Scotland. (pp. 316-323). Glasgow, Scotland: ICBPSA. (For this paper, the best student paper award was granted)


Appendices

A. Low-level TCP/IP sockets library

```c
#include <sys/types.h>
#include <sys/socket.h>
#include <netinet/in.h>
#include <netdb.h>
#include <string.h>
#include <unistd.h>
#include <stdio.h>
#include <stdlib.h>

#define SOCKET_ERROR        -1
#define BUFFER_SIZE         100
#define MESSAGE             "This is the message I'm sending back and forth"
#define QUEUE_SIZE          5
#define HOST_NAME_SIZE      21

/* Common block to hold socket IDs */
extern struct {
    int hsocket[40];
    int nhostport[40];
} skt_;

/* SOCKET SERVER OPEN*/
socketserveropen_(socketidp)
int *socketidp;
{
    int hServerSocket; /* handle to socket */
    struct hostent* pHostInfo; /* holds info about a machine */
    struct sockaddr_in Address; /* Internet socket address stuct */
    int nAddressSize=sizeof(struct sockaddr_in);
    int socketidpi;
    socketidpi=socketidp-1;
    printf("nMaking socket");
    /* make a socket */
    hServerSocket=socket(AF_INET,SOCK_STREAM,0);
    if(hServerSocket == SOCKET_ERROR)
    {
        printf("\nCould not make a socket.");
        return 0;
    }
    /* fill address struct */
    Address.sin_addr.s_addr=INADDR_ANY;
    Address.sin_port=htons(skt_.nhostport[socketidpi]);
    ```
Address.sin_family=AF_INET;

printf("\nBinding to port %d",skt_.nhostport[socketidpi]);
/* bind to a port */
/*if(bind(hServerSocket,(struct sockaddr*)&Address,sizeof(Address))
 == SOCKET_ERROR)*/

while(bind(hServerSocket,(struct sockaddr*)&Address,sizeof(Address))
 == SOCKET_ERROR){
    printf("\nCould not connect to host. Port \n", skt_.nhostport[socketidpi]);
    /*return 0;*/
    skt_.nhostport[socketidpi]=skt_.nhostport[socketidpi]+1;
    Address.sin_port=htons(skt_.nhostport[socketidpi]);
}
/* get port number */
getsockname( hServerSocket, (struct sockaddr *) &Address,(socklen_t *)&nAddressSize);
printf("opened socket as fd (%d) on port (%d) for stream i/o\n",hServerSocket,
ntohs(Address.sin_port));

printf("Server\n\tsin_family = %d\n\tsin_addr.s_addr = %d\n\tsin_port = %d\n",Address.sin_family
, Address.sin_addr.s_addr
, ntohs(Address.sin_port)
);
/* get port number to send it to main program */
skt_.nhostport[socketidpi]=ntohs(Address.sin_port);

printf("Making a listen queue of %d elements",QUEUE_SIZE);
/* establish listen queue */
if(listen(hServerSocket,QUEUE_SIZE) == SOCKET_ERROR)
{
    printf("\nCould not listen\n");
    return 0;
}

printf("\nWaiting for a connection\n");

skt_.hsocket[socketidpi]=accept(hServerSocket,(struct sockaddr*)&Address,(socklen_t *)
&nAddressSize);
    printf("\nGot a connection");
    printf("\nSocketumber:" %d \n",skt_.hsocket[socketidpi]);
}

/*________________________________________________________________________*/
/* SOCKET CLIENT OPEN*/

126
socketclientopen_(hostportfc,strHostNamef)
int *hostportfc;
char strHostNamef[HOST_NAME_SIZE];
{
    struct hostent *pHostInfo; /* holds info about a machine */
    struct sockaddr_in Address; /* Internet socket address struct */
    long nHostAddress;
    char pBuffer[BUFFER_SIZE];
    unsigned nReadAmount;
    int nhostportl;
    char strHostName[HOST_NAME_SIZE];

    /* Copy input parameters to new variables */
    nhostportl=*hostportfc;
    strcpy(strHostName,strHostNamef);

    printf("\nMaking a socket\n");
    /* make a socket */
    skt_.hsocket[1]=socket(AF_INET,SOCK_STREAM, IPPROTO_TCP);
    if(skt_.hsocket[1] == SOCKET_ERROR)
    {
        printf("\nCould not make a socket\n");
        return 0;
    }

    /* get IP address from name */
pHostInfo=gethostbyname(strHostName);
    /* copy address into long */
    memcpy(&nHostAddress,pHostInfo->h_addr,pHostInfo->h_length);

    /* fill address struct */
    Address.sin_addr.s_addr=nHostAddress;
    Address.sin_port=htons(nhostportl);
    Address.sin_family=AF_INET;

    printf("\nConnecting to %s on port %d:",strHostName,nhostportl);

    /* connect to host */
    if(connect(skt_.hsocket[1],(struct sockaddr*)&Address,sizeof(Address))
        == SOCKET_ERROR)
    {
        printf("\nCould not connect to host\n");
        return 0;
    }
}

/* SOCKET WRITE*/

socketwrite_(outvar, socketid)
float *outvar;
int *socketid;
{ char dummy1[100];
  int stringlenght;

  /*     usleep(6000000); */

  stringlenght=sprintf(dummy1,"%10.3e",*outvar);
  stringlenght=stringlenght+1;
  /*   printf("Sending [%s] with %d characters to Socket %d\n",dummy1,stringlenght,
       *socketid);*/
  /*    write variable to socket.*/

    write(*socketid,dummy1,stringlenght);
}

/*________________________________________________________________________*/
/* SOCKET READ*/
socketread_(invar, socketid)
  float *invar;
  int *socketid;
  {
    char dummy1[BUFFER_SIZE];
    char *pEnd;
    double dummy2;
    /*     usleep(6000000); */
    /*
    /* printf("Reading sockets on c: %d.\n",*socketid); */
    /* read variable to socket.*/
    read(*socketid,dummy1,BUFFER_SIZE);

    /*   printf("Variable received character format\"%s\n",dummy1); */
    dummy2=strtod(dummy1,&pEnd);
    /*   printf("Converted to double precision \"%10.3e\n",dummy2); */
    /*   *invar=dummy2;*/
    /*   printf("Converted to floating variable \"%10.3f\n",*invar); */
  }

/*________________________________________________________________________*/
/* SOCKET CLOSE*/
socketclose_(int socketid)
  {
    close(socketid);
  }
B. Examples of emulators for TCP/IP sockets server and client

program EMULATOR-client

C This routine tests ESP-r socket server for the coupling with HAMFEM.
   integer i,j

C Common block to hold socket IDs
   common/skt/hsocket(8)
   integer hsocket/8*-1/>

C Port number. Hardcoded.
   integer fnhostport(8)/8*52175/

C Servername
   character servername*21 /*bps01-net0.bwk.tue.nl*/

C Variables to be exchanged
   real tsi/20.0/, tso/10.0/, CCEHAM, CIEHAM, CCIHAM, CIIHAM, testcalc
   real testers, testerss

C Open the sockets and get socket ID
   call socketclientopen(fnhostport(8),servername)
   write (*,*) " 
   write (*,*) "Socket opened. Socket id." 
   write (*,*) hsocket(8)

   testers=0
   testerss=0

   j=365*24

   open(unit=8, file='receivedfromesp.txt')
   open(unit=9, file='sendtoesp.txt')

   do 999 i=1,j

   C Send information
      tsi=tsi !+0.001*i
      tso=tso !-0.001*i
      write (*,*) " "
      write (*,*) "Client sending information to the Server."
      call socketwrite(tsi,hsocket(8))
      call socketread(testers,hsocket(8))
      call socketwrite(tso,hsocket(8))
      write(9,'(F10.2,A,F10.2)') tsi,' ',tso

   C Read information
      write (*,*) " "
      call socketread(CCEHAM,hsocket(8))
      call socketwrite(testerss,hsocket(8))
      call socketread(CIEHAM,hsocket(8))
      call socketwrite(testersss,hsocket(8))

999 continue
call socketread(CCIHAM,hsocket(8))
call socketwrite(testerss,hsocket(8))
call socketread(CIIHAM,hsocket(8))
write (*,*) "Data received from the server."
testcalc=CCEHAM+CIEHAM+CCIHAM+CIIHAM
& CCEHAM,' ',CIEHAM,' ',CCIHAM,' ',CIIHAM,' ',testcalc
999   continue
   close(unit=8)
   close(unit=9)
C Close sockets
C    write (*,*) "Closing socket 
C    call socketclose(hsocket(8))
end

program EMULATOR-server
C This routine tests HAMFEM socket server for the coupling with ESP-r.
   integer i,j
C Common block to hold socket IDs
   common/skt/hsocket(8)
   integer hsocket/8*-1/
C Port number. Hardcoded.
   integer fnhostport(8)/8*50010/
C Servername
C   character servername*21 /"bps01-net0.bwk.tue.nl"/
C Variables to be exchanged
   real tsi(8736),tso(8736),CCEHAM(8736),CIEHAM(8736),CCIHAM(8736),CIIHAM(8736),testcalc
   real testers, testerss
C Open the sockets and get socket id
   call socketserveropen()
   write (*,*) "Socket opened"
   testers=0
testerss=0
   j=364*24
   open(unit=8,file='sendtohamfem.txt')
   open(unit=9,file='receivedfromhamfem.txt')
   CCEHAM(1)=-11.91;CIEHAM(1)=-66.72
CCEHAM(2)=-13.9;CIEHAM(2)=-58.89
CCEHAM(3)=-15.1;CIEHAM(3)=-22.7
CCEHAM(4)=-15.5;CIEHAM(4)=-14.72
...(these lines are omitted for brevity)

... 
CCIHAM(8729)=-7.17;CIIHAM(8729)=176.84
CCIHAM(8730)=-6.73;CIIHAM(8730)=139.53
CCIHAM(8731)=-6.28;CIIHAM(8731)=114.94
CCIHAM(8732)=-6.84;CIIHAM(8732)=119.51
CCIHAM(8733)=-7;CIIHAM(8733)=119.42
CCIHAM(8734)=-7.03;CIIHAM(8734)=117.76
CCIHAM(8735)=-7.05;CIIHAM(8735)=116.46
CCIHAM(8736)=-7.06;CIIHAM(8736)=116.01

do 999 i=1,j
    write (*,*) i
    C Send information
    tsi=0.001*i
    tso=0.001*i
    C write (*,*) " "
    C write (*,*) "Client sending information to the client."
    call socketread(tsi(i),hsocket(8))
    call socketwrite(testers,hsocket(8))
    call socketread(tso(i),hsocket(8))
    write(9,'(F10.2,A,F10.2)') tsi(i),' ',tso(i)

C Read information
C write (*,*) " "
    call socketwrite(CCEHAM(i),hsocket(8))
    call socketread(testerss,hsocket(8))
    call socketwrite(CIEHAM(i),hsocket(8))
    call socketread(testerss,hsocket(8))
    call socketwrite(CCIHAM(i),hsocket(8))
    call socketread(testerss,hsocket(8))
    call socketwrite(CIIHAM(i),hsocket(8))
    call socketread(testerss,hsocket(8))
C write (*,*) "Data received from the client."

testcalc=CCEHAM(i)+CIEHAM(i)+CCIHAM(i)+CIIHAM(i)
& CCEHAM(i),',',CIEHAM(i),',',CCIHAM(i),',',CIIHAM(i),',',testcalc

999 continue

    close(unit=8)
    close(unit=9)

C Close sockets

    write (*,*) "Closing socket."
    call socketclose(hsocket(8))
    write (*,*) "fakeserver complete"
end
C. Central intervals of IEA-ECBCS Annex 41 - Exercise 1B

The table below provides hourly data obtained after statistical treatment of results from IEA-ECBCS Annex 41 –Exercise 1-B, as described in Section 5.4 and shown in Figure 5.11, Figure 5.12 and Figure 5.13.

<table>
<thead>
<tr>
<th>Time (min-max)</th>
<th>T air (°C)</th>
<th>RH air (%)</th>
<th>T roof out (°C)</th>
<th>RH roof out (%)</th>
<th>Heating energy demand (Wh)</th>
<th>Cooling energy demand (Wh)</th>
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<tbody>
<tr>
<td>1</td>
<td>19.9-20.4</td>
<td>42.9-53.9</td>
<td>11.4-13.2</td>
<td>66.3-79.3</td>
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<td>43.2-53.0</td>
<td>10.9-12.8</td>
<td>70.2-82.1</td>
<td>322-722</td>
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<td>10.5-12.3</td>
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<td>750-1007</td>
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<td>10.7-12.0</td>
<td>75.0-83.2</td>
<td>927-1293</td>
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<td>845-1212</td>
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<td>42.1-50.6</td>
<td>22.7-26.7</td>
<td>37.5-47.8</td>
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<td>41.3-46.9</td>
<td>27.0-31.3</td>
<td>28.8-35.0</td>
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</tr>
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<td>41.0-48.6</td>
<td>23.1-25.9</td>
<td>25.5-32.0</td>
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<td>19.8-22.5</td>
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<td>44.6-55.8</td>
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</table>
D. List of modifications in ESP-r source code

This appendix lists the files modified in ESP-r source code for the implementation of one-way coupling using flux equations and two-way loose coupling. In each file, the main operations regarding BES-BEHAM coupling are listed as well. Files names and locations are shown in bold, while subroutines are underscored.

**esrubps/simcon.F**

**SIMCON**
- define surfaces to be coupled (hardcoded)
- open sockets and wait for HAMFEM reply
- open files to store received and sent information
  - CALL MZNUMA
- close socket

**MZTRAC**
- Add trace facility of flux equation for one-way coupling

**esrubps/bmatsv.F**

**MZNUMA**
- CALL MZCOE3 (post processing of coupling)
- CALL MZSETU
- CALL MZVAPC
- Reduce the number of wall
  - CALL MTXCTL (solve matrix – not modified)
- Restore nodes ID, assign temperature to proper nodes
- Restore the number of wall
- Restore matrixes (W matrix, E matrix)
- Read values from HAMFEM
- Assign values calculated by HAMFEM
  - CALL SURBAL (send values to HAMFEM)
esrubld/bmatsu.F

MZSETU
Modify matrixes (W matrix, E matrix) excluding coupled walls (lines and columns in matrix E) and multiplying coefficients in matrix E

esrubld/subsys.F

MZVAPC
Calculate the terms of moisture flux equation
Include moisture flux from the wall into the zone moisture balance
Define moisture source profile (hardcoded)

esrubld/blibsv.F

SURBAL
Calculate the terms of heat flux equation
Send values of heat and moisture to HAMFEM
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