



# International Energy Agency, EBC Annex 68

# Indoor Air Quality Design and Control in Low-Energy Residential Buildings

Subtask 3: Modelling of Energy Efficiency and IAQ -Review, Gap analysis and Categorization

# Energy in Buildings and Communities Technology Collaboration Programme October 2020



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# **Energy in Buildings and Communities Programme**

October 2020

# Editors

John Grunewald, Dresden University of Technology, Germany (john.grunewald@tu-dresden.de)

# **Contributing Authors**

John Grunewald, Dresden University of Technology, Germany (john.grunewald@tu-dresden.de) Jianshun Zhang, Syracuse University, USA (jszhang@syr.edu) Andreas Nicolai, Dresden University of Technology, Germany (andreas.nicolai@tu-dresden.de) Dirk Weiß, Dresden University of Technology, Germany (dirk.weiss@tu-dresden.de) Stephan Hirth, Dresden University of Technology, Germany (stephan.hirth@tu-dresden.de) Jia Zile, Dresden University of Technology, Germany (jiazile2010@gmail.com) Jakub Kolarik, Technical University of Denmark, Denmark (jakol@byg.dtu.dk) Gabriel Rojas-Kopeining, University of Innsbruck, Switzerland (Gabriel.Rojas-Kopeinig@uibk.ac.at) Klaas De Jonge, Ghent University, Belgium ((Klaas.DeJonge@UGent.be)) Ben Krämer, RWTH Aachen University, Germany (kraemer@e3d.rwth-aachen.de)

# **Reviewed by**

Gabriel Rojas-Kopeining, University of Innsbruck, Switzerland (Gabriel.Rojas-Kopeinig@uibk.ac.at) Nathan Mendes, Pontifical Catholic University of Paraná, Brazil (nathan.mendes@pucpr.br)

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### Preface

#### The International Energy Agency

The International Energy Agency (IEA) was established in 1974 within the framework of the Organisation for Economic Co-operation and Development (OECD) to implement an international energy programme. A basic aim of the IEA is to foster international co-operation among the 30 IEA participating countries and to increase energy security through energy research, development and demonstration in the fields of technologies for energy efficiency and renewable energy sources.

#### The IEA Energy in Buildings and Communities Programme

The IEA co-ordinates international energy research and development (R&D) activities through a comprehensive portfolio of Technology Collaboration Programmes. The mission of the IEA Energy in Buildings and Communities (IEA EBC) Technology Collaboration Programme is to develop and facilitate the integration of technologies and processes for energy efficiency and conservation into healthy, low emission, and sustainable buildings and communities, through innovation and research. (Until March 2013, the IEA EBC Programme was known as the IEA Energy Conservation in Buildings and Community Systems Programme, ECBCS.)

The R&D strategies of the IEA EBC Programme are derived from research drivers, national programmes within IEA countries, and the IEA Future Buildings Forum Think Tank Workshops. These R&D strategies aim to exploit technological opportunities to save energy in the buildings sector, and to remove technical obstacles to market penetration of new energy efficient technologies. The R&D strategies apply to residential, commercial, office buildings and community systems, and will impact the building industry in five areas of focus for R&D activities:

- Integrated planning and building design
- Building energy systems
- Building envelope
- Community scale methods
- Real building energy use

#### The Executive Committee

Overall control of the IEA EBC Programme is maintained by an Executive Committee, which not only monitors existing projects, but also identifies new strategic areas in which collaborative efforts may be beneficial. As the Programme is based on a contract with the IEA, the projects are legally established as Annexes to the IEA EBC Implementing Agreement. At the present time, the following projects have been initiated by the IEA EBC Executive Committee, with completed projects identified by (\*) and joint projects with the IEA Solar Heating and Cooling Technology Collaboration Programme by  $(\clubsuit)$ :

- Annex 1: Load Energy Determination of Buildings (\*)
- Annex 2: Ekistics and Advanced Community Energy Systems (\*)
- Annex 3: Energy Conservation in Residential Buildings (\*)
- Annex 4: Glasgow Commercial Building Monitoring (\*)
- Annex 5: Air Infiltration and Ventilation Centre
- Annex 6: Energy Systems and Design of Communities (\*)
- Annex 7: Local Government Energy Planning (\*)
- Annex 8: Inhabitants Behaviour with Regard to Ventilation (\*)
- Annex 9: Minimum Ventilation Rates (\*)
- Annex 10: Building HVAC System Simulation (\*)
- Annex 11: Energy Auditing (\*)
- Annex 12: Windows and Fenestration (\*)
- Annex 13: Energy Management in Hospitals (\*)
- Annex 14: Condensation and Energy (\*)
- Annex 15: Energy Efficiency in Schools (\*)
- Annex 16: BEMS 1- User Interfaces and System Integration (\*)
- Annex 17: BEMS 2- Evaluation and Emulation Techniques (\*)
- Annex 18: Demand Controlled Ventilation Systems (\*)

- Annex 19: Low Slope Roof Systems (\*)
- Annex 20: Air Flow Patterns within Buildings (\*)
- Annex 21: Thermal Modelling (\*)
- Annex 22: Energy Efficient Communities (\*)
- Annex 23: Multi Zone Air Flow Modelling (COMIS) (\*)
- Annex 24: Heat, Air and Moisture Transfer in Envelopes (\*)
- Annex 25: Real time HVAC Simulation (\*)
- Annex 26: Energy Efficient Ventilation of Large Enclosures (\*)
- Annex 27: Evaluation and Demonstration of Domestic Ventilation Systems (\*)
- Annex 28: Low Energy Cooling Systems (\*)
- Annex 29: 🔅 Daylight in Buildings (\*)
- Annex 30: Bringing Simulation to Application (\*)
- Annex 31: Energy-Related Environmental Impact of Buildings (\*)
- Annex 32: Integral Building Envelope Performance Assessment (\*)
- Annex 33: Advanced Local Energy Planning (\*)
- Annex 34: Computer-Aided Evaluation of HVAC System Performance (\*)
- Annex 35: Design of Energy Efficient Hybrid Ventilation (HYBVENT) (\*)
- Annex 36: Retrofitting of Educational Buildings (\*)
- Annex 37: Low Exergy Systems for Heating and Cooling of Buildings (LowEx) (\*)
- Annex 38: 🔅 Solar Sustainable Housing (\*)
- Annex 39: High Performance Insulation Systems (\*)
- Annex 40: Building Commissioning to Improve Energy Performance (\*)
- Annex 41: Whole Building Heat, Air and Moisture Response (MOIST-ENG) (\*)
- Annex 42: The Simulation of Building-Integrated Fuel Cell and Other Cogeneration Systems (FC+COGEN-SIM) (\*)
- Annex 43: 🌣 Testing and Validation of Building Energy Simulation Tools (\*)
- Annex 44: Integrating Environmentally Responsive Elements in Buildings (\*)
- Annex 45: Energy Efficient Electric Lighting for Buildings (\*)
- Annex 46: Holistic Assessment Tool-kit on Energy Efficient Retrofit Measures for Government Buildings (EnERGo) (\*)
- Annex 47: Cost-Effective Commissioning for Existing and Low Energy Buildings (\*)
- Annex 48: Heat Pumping and Reversible Air Conditioning (\*)
- Annex 49: Low Exergy Systems for High Performance Buildings and Communities (\*)
- Annex 50: Prefabricated Systems for Low Energy Renovation of Residential Buildings (\*)
- Annex 51: Energy Efficient Communities (\*)
- Annex 52: 🌣 Towards Net Zero Energy Solar Buildings (\*)
- Annex 53: Total Energy Use in Buildings: Analysis and Evaluation Methods (\*)
- Annex 54: Integration of Micro-Generation and Related Energy Technologies in Buildings (\*)
- Annex 55: Reliability of Energy Efficient Building Retrofitting Probability Assessment of Performance and Cost (RAP-RETRO) (\*)
- Annex 56: Cost Effective Energy and CO2 Emissions Optimization in Building Renovation (\*)
- Annex 57: Evaluation of Embodied Energy and CO2 Equivalent Emissions for Building Construction (\*)
- Annex 58: Reliable Building Energy Performance Characterisation Based on Full Scale Dynamic Measurements (\*)
- Annex 59: High Temperature Cooling and Low Temperature Heating in Buildings (\*)
- Annex 60: New Generation Computational Tools for Building and Community Energy Systems (\*)
- Annex 61: Business and Technical Concepts for Deep Energy Retrofit of Public Buildings (\*)
- Annex 62: Ventilative Cooling (\*)
- Annex 63: Implementation of Energy Strategies in Communities (\*)
- Annex 64: LowEx Communities Optimised Performance of Energy Supply Systems with Exergy Principles (\*)
- Annex 65: Long-Term Performance of Super-Insulating Materials in Building Components and Systems (\*)
- Annex 66: Definition and Simulation of Occupant Behavior in Buildings (\*)
- Annex 67: Energy Flexible Buildings
- Annex 68: Indoor Air Quality Design and Control in Low Energy Residential Buildings
- Annex 69: Strategy and Practice of Adaptive Thermal Comfort in Low Energy Buildings
- Annex 70: Energy Epidemiology: Analysis of Real Building Energy Use at Scale

- Annex 71: Building Energy Performance Assessment Based on In-situ Measurements
- Annex 72: Assessing Life Cycle Related Environmental Impacts Caused by Buildings
- Annex 73: Towards Net Zero Energy Resilient Public Communities
- Annex 74: Competition and Living Lab Platform
- Annex 75: Cost-effective Building Renovation at District Level Combining Energy Efficiency and Renewables
- Annex 76: Coper Renovation of Historic Buildings Towards Lowest Possible Energy Demand and CO<sub>2</sub> Emissions
- Annex 77: 🌣 Integrated Solutions for Daylight and Electric Lighting
- Annex 78: Supplementing Ventilation with Gas-phase Air Cleaning, Implementation and Energy Implications
- Annex 79: Occupant -Centric Building Design and Operation
- Annex 80: Resilient Cooling
- Annex 81: Data-Driven Smart Buildings
- Working Group Energy Efficiency in Educational Buildings (\*)
- Working Group Indicators of Energy Efficiency in Cold Climate Buildings (\*)
- Working Group Annex 36 Extension: The Energy Concept Adviser (\*)
- Working Group HVAC Energy Calculation Methodologies for Non-residential Buildings
- Working Group Cities and Communities
- Working Group Building Energy Codes
- Working Group International Building Materials Database

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# **Summary**

Existing knowledge is still inadequate for predicting the combined effects of building energy performance and indoor air quality. This concerns strategies for optimal HVAC system operation, the hygrothermal conditions of the building envelope, thermal comfort in zones and the chemical reactions on various types and concentrations of indoor pollution. In light of most recent revelation of the importance of secondary emissions such as Ozone-initiated indoor air and surface chemistry, a modelling approach of the effects of combined heat, air, moisture and pollutant (CHAMPS) transport and their impact on energy and IAQ is targeted in ST3.

Since many building performance simulation tools already exist, the focus in ST3 is NOT the development of a new overall model. Instead, the focus is on interoperability of existing models and development of quality assurance criteria for optimal use of these tools. Therefore, the main target of ST3 is a review, gap analysis and categorization of existing models and standards.

**Strategies for ensuring quality** in building performance simulation include supporting actions as common exercises and a collaborative development towards a fully coupled CHAMPS modeling platform. This platform will be an open-source repository for numerical solvers and data being able to capture the most important physical processes involved. This platform will be the basis for a seamless continuation of the modeling activities of the IEA EBC Annexes – especially it will build upon the achievements of the Annex 60, an effort on "New generation computational tools for building and community energy systems based on the Modelica and Functional Mock-up Interface standards". The most important aspects are:

- Broad and hierarchically organized modeling scope
  - Most important CHAMPS aspects to be captured
  - Different levels of detail (walls, rooms, buildings, district)
  - Gradual buildup of model complexity
- Commonly agreed reference solutions
  - Participation of commonly used tools
  - Model-to-model comparison (comparison with measured data is not planned)
  - o Fully documented input data including project files
- Interoperability and performance
  - Test of different coupling technologies
  - o Test of large problems on reasonable execution time
  - Test of numerical robustness
- Towards fully automated quality assurance checks
  - Automatic execution of test cases
  - Automated evaluation of results
  - o Automatically generated reports and messaging system

In ST3, these targets are approached by definition of a common exercise based on the PASSYS Cells Project. We use hygrothermal envelope simulations tools (2D) as well as whole building energy performance simulation tools (3D) during this exercise. We consider heat, air, moisture and VOC flows, coupled walls and rooms and a gradual buildup of model complexity by a series of test cases.

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# Appendix 1: 2D Simulation results

Appendix 2: 3D Simulation results

# **1** Introduction

### 1.1 About IEA EBC Annex 68

The overall objective of the IEA EBC Annex 68 is to provide a scientific basis usable for optimal and practically applicable design and control strategies for **better Indoor Air Quality (IAQ)** in residential buildings. These strategies are intended to ensure minimal possible energy use. The aim of Annex 68 is to gather the existing data and provide new data on pollution sources in buildings, to model the indoor hygrothermal conditions, air quality and thermal systems, and to find the methods to optimize ventilation and air-conditioning. Annex 68 is focused on **low-energy residential buildings**.

There are numerous different national definitions and concepts describing low-energy buildings. Some, for example, focus on the renewable energy production on-site (Blomsterberg et al., 2012) and discuss not only the reduction of energy use. All definitions have in common that a low-energy building should achieve better or significantly better energy performance compared to a traditional contemporary building practice to reduce the use of fossil fuels such as oil, gas and coal (Thullner, 2010). In some countries or regions, low-energy buildings are defined by the building codes or in relation to the energy standard. It may happen that one building, which can be classified as low-energy in one country, use more energy than a standard building in another country. Also, standards have improved with time and the low-energy standards from the past are likely to be standards today (Laustsen, 2008). In the present project, a building is considered as low-energy when it has a better energy performance than the typical new building following the minimum standards defined in building regulations at a given point of time in a given country.

The work of the Annex 68 is organized in five subtasks (Figure 1): **Subtask 1** is setting up the metrics to assess the performance of low-energy buildings as regards indoor air quality combining the aspirations to achieve very high energy performance without compromising indoor environmental quality. **Subtask 2** is gathering the existing knowledge and providing new data about indoor air pollutants in relation to combined heat, air and moisture transfer. **Subtask 3** is identifying and developing modelling tools that can assist designers and managers of buildings in accounting for IAQ. **Subtask 4** is developing design and control strategies for energy efficient ventilation in residential buildings that will not lessen indoor air quality. **Subtask 5** is conducting field measurements to examine and optimize different control and design strategies.



Figure 1: Schematic overview of the subtasks in Annex 68 and their interrelations. Solid lines indicate direct relations; dotted lines indicate indirect ones.

# 1.2 Outline of the work under Subtask 3

The work in ST3 focused on selected activities, which were discussed and agreed among the participants. The outcome of the work is described by the list of deliverables.

### 1.2.1 Activities

- Literature survey and provision of knowledge about contemporary modelling capabilities in whole building energy and hygrothermal analysis in combination with airflow and emission models
- Definition of selection criteria for models in order to establish a platform of tools
- Development of a paradigm for work with these models by definition of reference cases with focus on specific physical/chemical processes/effects in the field of building energy performance under high IAQ conditions
- Identification of gaps in current modelling capabilities: The gap analysis will be translated into recommendations for further development/interfacing of tools. This activity includes incorporation of the methods for analysis in modelling paradigms from other IEA activities, e.g. IEA Annex 60.
- Development of new input to standards for quality assurance of modelling tools, when and if necessary, that will be needed to model the interaction between energy efficient operation and high IAQ
- Recommendation of a modelling framework with necessary components for evaluating the energy and IAQ performance various design and operation strategies

#### 1.2.2 Deliverables

- 1. Overall analysis of the practice integration of building performance simulation tools
- 2. Reference cases with problem description, input parameters and solution (Common Exercise)
- 3. Classification of available tools according to their strengths and weaknesses
- 4. Feature requests and implementations from the gap analysis of available tools
- 5. Proposals for improvement of quality assurance standards
- 6. A project report and referenced journal papers

#### 1.2.3 Stakeholders involved

Apart from partners from academia, major software vendors and engineering enterprises have a vital interest in these activities and companies/research teams involved in building design tool development have contributed to the subtask.

# **1.3 Organization of the final report**

In Chapter 2 of this report, we identify the challenges encountered in practice regarding integrated modeling and analysis throughout the life-cycle of buildings design, construction, operation and re-use and demolition. Based on a broad review of the tools currently available, knowledge and tool gaps are identified and discussed. Emphasis is given to tools for workflow integration, life-cycle cost analysis as well as integrated consideration and modeling of different performance aspects such as energy efficiency, thermal comfort, IAQ, and cost during building design and operation. A detailed review and discussion then follow in Chapter 3 regarding various integration tools available, giving particular emphasis to Modelica and CHAMPS simulation platforms and functional mock-up interface as an approach for integration of disciplinary simulation tools. An approach and platform for enhancing knowledge transfer from research to practice is also suggested. As accuracy and reliability of the modeling and simulation tool is vital for their wide applications, in Chapter 4, we present model validation results from a series of common excises cases for simulation from simple to increasingly complicated scenarios, which helps to identify the limitations of existing simulation tools. In Chapter 5, we described the methods and results to address the some of the limitations identified including new implementations in the CHAMPS platform to include new VOC simulation capabilities coupled with heat and moisture simulations, and new development on the similarity theory between moisture and VOC transport in porous media. In Chapter 6, we further propose a quality assurance protocol and platform for continuing the common excises to validate simulation tools through international multi-institution collaboration. This is followed by a summary of the major findings from subtask 3 and recommendations for future studies in Chapter 7.

# 2 Challenges in practice integration and gap analysis

# 2.1 Introduction

The current trends in energy supply and use are obviously unsustainable in economic, ecological and social terms. Without decisive action, the 2050 targets for global greenhouse gas emissions will not be met, and increased demand will raise concerns about security of supply (Agency, 2011). This situation has to be changed in a revolutionary way. One of the greatest challenges of the 21st century is to ensure a reliable, economically affordable and environmentally friendly energy supply and use system. Although the exact ratios vary in different countries and under different conditions, it is known that the construction sector consumes about a third of the total energy consumption. The urgency and importance of the energy transition in the construction sector is self-evident.

Energy efficiency, renewable energy and low-carbon energy technologies are all accepted concepts in the construction industry today. Many innovative technologies have been implemented and many pilot projects have been carried out as a demonstration around the world. The European Horizon  $2020^1$  is the biggest EU Research and Innovation Programme ever with nearly &80 billion of funding available over 7 years (2014 to 2020) – in addition to the private investment that this money will attract. Efforts were made in Germany within the framework of projects funded by the Federal Ministry for Economic Affairs and Energy and now bundled in the Research Network "Energiewendebauen"<sup>2</sup>.





There is no doubt that the purpose of the building and the building system operation is to create an adequate living and working environment for humans. Modern people spend a lot of time in buildings. An adequate indoor climate for humans is the most important criterion for a qualified shelter. The satisfaction and productivity of the occupants in the workplace strongly depends on indoor thermal comfort and indoor air quality (IAQ). In other words, human well-being is a critical aspect and should be a priority factor to consider when building and renovating buildings.

It is clear that energy savings and indoor comfort are somehow contradictory (Figure 2). In addition, three sub-factors of indoor human comfort can conflict and compete with one another: thermal comfort, visual

<sup>&</sup>lt;sup>1</sup> European Horizon 2020 website: <u>https://ec.europa.eu/programmes/horizon2020/en/what-horizon-2020</u>

<sup>&</sup>lt;sup>2</sup> Research Network "Energiewendebauen": <u>https://www.forschungsnetzwerke-energie.de/energiewendebauen</u>

comfort, and indoor air quality. Take as an example the air conditioning in a hot summer. Each degree of lowered temperature causes increased energy consumption and a correspondingly high electricity bill. To compromise indoor air quality and human health to save energy is a typical example of how this problematic situation is not adequately addressed.

The relationship between the building and its surroundings must also be considered carefully. Passive principles such as sun and wind orientation and envelope characteristics are closely related to building performance and have been carefully considered over the past millennia. Unfortunately, after the invention and widespread use of modern HVAC systems, designers began to ignore all passive principles and simply use high-performance HVAC equipment to maintain the desired indoor climate. A typical example is the glass facade construction in the Middle East. Of course, this inappropriateness of buildings with the environment definitely causes a tremendous waste of energy.

As existing buildings become more complex and integrated, conflicts and integrated requirements for the design and operation of buildings must be considered. The established building standards listed in Table 1 are illustrative explanations of this complexity and integration. In addition to regulating energy consumption, thermal comfort, health issues, acoustics and visual comfort are all or part of these building standards to govern building design, construction and operation.

#### Table 1: Building energy and environmental standards

Code and full name
LEED-Leadership in Energy and Environmental Design
EPBD-Energy Performance of Buildings Directive
BREEAM-Building Research Establishment Environmental Assessment Methodology
JGJ/T288-Standard for building energy performance certification
CASBEE-Comprehensive Assessment System for Built Environment Efficiency

The planning and optimization of increasingly complex and flexible buildings, especially with regard to integrated or even conflict-related requirements, must be carried out properly. Appropriate design and operation methods, data and tools are essential.

Most of the current building simulation tools are the results of funded projects for specific research purposes. Typically, these tools are developed in research organizations and used by the organization's employees rather than by designers and engineers. In financial and intellectual terms, this is definitely a waste, as designers and engineers have to deal with complex issues in construction practice and certainly need the support of building simulation tools. The general aim is to promote the use of simulation tools not only by simulation experts for research purposes, but also by designers and engineers in practical work.

As well-designed tools can only be identified on the basis of an adequate requirement analysis, the focus initially is on meeting the requirements of engineers in practice when planning and operating buildings. The development of a multi-criteria analysis, integration of the entire life cycle, interdisciplinary interaction, controlled integration / optimization together with the influence of "Industry 4.0" in the construction discipline are discussed in turn. This is not just an enumeration of emerging scenarios, but also an exploration

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to find out that interdisciplinary integration is of increasing importance as buildings become more advanced and complex.

The multi-criteria analysis shows that designers and engineers must at least simultaneously consider energy efficiency and initial costs. Human well-being, environmental impact and lifecycle costs are also affected. However, current workflows and cooperation mechanisms between different simulation tools cannot adequately meet the requirements for analyzing multiple criteria in the design and operation of buildings. Further detailed discussions on energy and cost simulation, energy and thermal comfort simulation, and control-related simulations suggest that construction practice is increasingly integrated, but that simulation capabilities are still inadequate and isolated. Therefore, related instruments need to be coordinated and linked from a socio-technical point of view to support the construction practice eventually.

Recent developments in the Modelica multi-domain modeling language (Hilding, Otter, & Mattsson, 2012) and the Functional Mock-up Interface (FMI) standard<sup>3</sup> have provided an efficient solution for both integration and practical use. Publicly available and freely usable frameworks and associated cooperation mechanisms are proposed. Individual models and tools could be coupled by co-simulation or model exchange according to the FMI standard. Together with complete and accurate databases, the integrated tools could be jointly validated and documented and then transferred to commercial partners for further improvement of usability, marketing and sale. In this way, a collaborative framework for knowledge transfer from research to practice could be created to adequately address integrated requirements issues and the use of research-oriented tools could be intensified in industrial construction practice.

Interoperability, technical standards and workflow protocol, these general terms for cooperative simulation development, are discussed further. The individual model quality is a fundamental guarantor for successful cooperative simulation systems. The cooperative development of Modelica libraries<sup>4</sup> is taken as an example to illustrate the problems involved and their solutions from both detailed technical and generalized sociotechnical perspectives.

### 2.2 A brief history of building performance simulation

In the past, the relevant knowledge and solutions could only be gained through experience and lessons learned from mistakes. Nowadays, this situation has changed dramatically with the development of information and computing technologies. Before the actual construction of a building, people can gain knowledge and detailed information about a building through simulation. The ability to simulate the future performance of a building or specific components offers designers and engineers the ability to test a range of options, balance competing requirements, and avoid potential problems.

The early development of building simulation tools focused primarily on the analysis of the thermal performance of buildings. During the HVAC design process, engineers need to calculate the peak load to determine the type and performance of the HVAC equipment. Before the introduction of the building simulation, the peak load calculation was performed by the HVAC engineers in the form of a manual

<sup>&</sup>lt;sup>3</sup> FMI standard website: <u>https://www.fmi-standard.org</u>

<sup>&</sup>lt;sup>4</sup> Modelica libraries website: <u>https://www.modelica.org/libraries</u>

calculation. With the development of computer technology in the construction industry, computerized tools can more efficiently and conveniently calculate the energy load.

In fact, it is the symbol of modern science and technology to rely more on analytical calculations, experiments and simulations than experience to develop and gather knowledge. The development of computer-aided building simulation over half a century has resulted in a wide range of currently available products. There is an online directory<sup>5</sup> for building energy simulation tools that was previously sponsored by the US Department of Energy and has now been adopted by IBPSA-USA (Figure 3). This directory contains information on more than 450 building software tools for assessing energy efficiency, renewable energy use and indoor sustainability. The building simulation tools listed in this directory include databases, spreadsheets, component and system analyzes, and energy performance simulation programs for buildings.



#### Figure 3: Screenshot of the IBPSA Building Energy Software Tools (BEST) directory

With the ability to predict the performance of a non-existent building, researchers and developers are soon no longer satisfied with simply replacing the hand calculation in the design process. Building simulation tools provide accurate information about buildings and / or building services, helping engineers and designers improve understanding. This also gives better opportunities to improve the quality and cost-effectiveness of buildings and building services. Therefore, more and more building simulation tools are being developed. As the number of tools increases, so has the scope of study objects in recent decades.

<sup>&</sup>lt;sup>5</sup> Building Energy Software Tools (BEST) directory: <u>https://www.buildingenergysoftwaretools.com</u>

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Today, apart from hourly peak load or annual energy consumption calculations, many other issues such as HVAC models and their control systems, coupled heat and mass transfer, air flow, indoor air quality, visual performance, acoustic performance, energy economy and renewable energy are the subject of evaluation by a variety of specialized or generalized simulation tools.

Enormous intelligence and financial resources have been invested in the creation of simulation codes and tools. Numerous design, modeling, and simulation work has been done using a variety of building simulation tools covering all building-related disciplines and areas.

Compared to simulation tools used in other industrial disciplines such as mechanical engineering, most building simulation tools are considered as in-house software. The term "in-house" implies that the software is developed in an organization and used only by the organization's employees and not by outside employees. It's probably the same group of people who develop and use specific "in-house" software for a particular project or series of projects. In other words, "in-house" software is used by researchers as a research tool rather than an engineering tool used by designers and engineers in the field.

Of course, simulation tools are required for the construction practice. However, most existing building simulation tools remain at the research level or "in-house" level and are not widely used in construction practice. In the following, this "research and application gap" will be discussed under both building design and operational perspectives to describe this disparity in detail.

### 2.3 Building energy simulation in practice

#### 2.3.1 Separate simulation work groups

Energy efficient construction or any other good quality building starts with a suitable design. The ideal method is to incorporate a building simulation tool to support the design process from the start, as the earlier optimization with building simulation tools will result in a better design and thus better energy efficiency of the building.



Figure 4: Current workflow of building design

However, as shown in Figure 4, the building simulation is somewhat separate from the planner's work process. In current construction practice, planners are not usually the users of building simulation tools. Simulation experts from different work groups or even different companies have to be employed to perform the simulation and propose optimized building solutions. For example, in the HVAC design process, HVAC engineers must first provide design information such as the type and characteristics of the devices. Subsequently, HVAC simulation experts perform modeling and simulation work, and HVAC engineers optimize

their schema based on simulation results. As other groups need to be involved in this process apart from the designers, additional coordination and consequently additional time and costs are inevitable.

In addition to the problem of separation of workgroups, there are also problems with data transformation for simulation groups: simulation experts often need to create models from scratch. This means that simulation models, especially HVAC models, are not automatically generated based on the designer's frequently used CAD (Computer Aided Design) file, and simulation experts must enter all design data manually. In summary, the building design process is still not fully supported by the simulation tools.

Someone may argue why one should worry about the separation between building design and simulation, as building simulation tools are traditionally not widely used in the construction industry. However, when compared to the application of simulation tools in other disciplines such as mechanical engineering or electrical engineering, it becomes clear that the integration of building simulation tools in construction is taking place with an extraordinary delay. The digitization and the R&D spending in construction run well behind other industries<sup>6</sup>. The question is asked whether the construction sector is ripe for disruption (Ernstsen, Maier, Larsen, & Thuesen, 2018).

Design objective	Industry field	Method description	
HV/AC aquinment	Building	HVAC designer cooperates with simulation expert	
nvac equipment		HVAC designer alone without simulation	
HVAC control	Control	Control designer alone with simulation	

#### Table 2: Comparison of application modes in building and control industries

An example is given in Table 2 to demonstrate this lagged situation by comparing the design process of the HVAC system with the design process of the HVAC device control system. The HVAC system design can definitely benefit from a detailed HVAC system simulation. HVAC designers could work with simulation experts to improve their design. However, most of them still work with an old-fashioned method that was implemented decades ago: they only calculate the peak value to determine the equipment capacity. Although HVAC designers are willing to work with simulation experts, this is a tedious process anyway.

In contrast to this situation, it is usually the same group of people that designs and simulates the behavior of the control system with simulation software such as MATLAB. Optimization with simulation is an unavoidable process when designing control systems. Simulation-aided tools are already widely used in the control industry.

#### 2.3.2 HVAC system and control system simulation

The HVAC system and control system should be simulated together as they always work together to perform their functions in modern buildings. However, there is an enormous gap concerning coupling between HVAC

<sup>&</sup>lt;sup>6</sup> See pdf version of the McKinsey report "The Construction Industry is Ripe for Disruption" available from: <u>https://www.mckinsey.com/~/media/McKinsey/Industries/Capital%20Projects%20and%20Infrastructure/Our%20In</u> <u>sights/Imagining%20constructions%20digital%20future/The-construction-industry-is-ripe-for-disruption-infographic.ashx</u>

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and control simulation that also applies more generally to building/HVAC and control, i.e. it is not only HVAC but also building simulation that can benefit from a simulation with detailed building control. The HVAC simulation and control simulation are now actually two relatively independent fields. An intuitive impression of this situation is shown in Figure 5.



Figure 5: Workflow of HVAC&Control system design and operation

The HVAC simulation developed by the HVAC engineer uses a detailed equipment model and simplified and limited control algorithms. Conversely, control engineers combine a detailed control model and a black box or simplified equipment model to simulate the behavior of control and HVAC equipment. It is easier and more convenient to establish a reasonable understanding by comparison between the control simulation tool, e.g. MATLAB and the building simulation tool, e.g. TRNSYS. The MATLAB/Simulink based building modelling library "CARNOT"<sup>7</sup> allows the combined simulation of building/HVAC and control, but is still not widely used.

Perspectives	HVAC part	Control part	Application
HVAC simulation	Detailed equipment	Simplified and limited control	HVAC system optimization and modification
Control simulation	Black box or simplified equipment	Detailed control	Simulation assisted control, FDD
Integrated practice	Detailed equipment	Detailed control	Characteristic of real building control; rarely observed in practice

#### Table 3: Enumeration of HVAC&Control model combinations

On the one hand, as a widely used tool in the control industry, MATLAB is able to model and simulate complex control algorithms and their reality control processes, but with extremely limited and simple ways to describe equipment. On the other hand, TRNSYS, which has a strong ability to model complex HVAC systems and limited control modeling capabilities. The ability to model multi-zone buildings with the Type 56 model and most basic control functions, and even part of the advanced control algorithm, have made TRNSYS a well-known and well-established tool for a long time. However, there is no way to conveniently model advanced and complex control algorithms such as neural networks, fuzzy logic, and genetic algorithms already implemented in construction practice.

<sup>&</sup>lt;sup>7</sup> A reference to the CARNOT toolbox is given at: <u>http://ibpsa-germany.org/wordpress/tools</u>

In general, control engineers and HVAC engineers have developed and expanded building management terminology in two different ways. Control engineers are mainly interested in whether the regulated target meets the control algorithm. The interest of the HVAC engineers is whether the HVAC equipment offers heating / cooling functions. Detailed control methods are not a priority of HVAC engineers. Although there are certain collaborations between these two groups, it is only a small effort rather than a full collaboration between two disciplines. Their individual development efforts in their own disciplines lead to this division situation for the building simulation.

In reality, many buildings are still poorly controlled due to incorrect setpoints, incorrect Proportional-Integral-Differential-Controller (PID) settings, lack of coordination of individual control loops, and other practical issues. Optimization with simulation can certainly help. Regardless of whether tools come from the control area or come from the construction sector, they cannot fully reflect the reality and fulfill the current practical requirements. Obviously, a combination of detailed HVAC and detailed control is required in any case. As more and more integrating questions emerge, the integration and the overall simulation should react much faster.

Control engineers, HVAC engineers, and simulation tool manufacturers have made significant contributions to building simulation, but the construction practice is not yet fully satisfactory. The future control simulation plays an increasingly important role both inside and outside the building simulation. Since control is the most important aspect in a coordinated large system, a small lack of control simulation can cause huge problems and they must be handled properly.

Project	Name	References
Annex 17	Building Energy Management Systems - Evaluation and Emulation Techniques	(Mansson & McIntyre, 1997)
Annex 25	Real Time HVAC Simulation	(Hyvärinen & Kärki, 1996)
Annex 34	Computer Aided Evaluation of HVAC System Performance	(Jagpal, 2006)
Annex 40	Commissioning of Building HVAC Systems for Improved Energy Performance	(Visier, 2003)
Annex 60	New Generation Computational Tools for Building & Community Energy Systems	(Wetter, van Treeck, & Hensen, 2013)
Annex 66	Definition and Simulation of Occupant Behavior in Buildings	(Yan & Hong, 2014)

Table 4: List of Annex programs for HVAC&Control and occupant simulation

In building operation, there is the challenge of getting the HVAC systems to work with maximum efficiency through appropriate control. However, the HVAC system of a building can only work as well as its control scheme works. If the importance of operation is neglected, an inappropriate control scheme can undo all the benefits or improvements of an excellent system design. In contrast, a good control scheme can significantly improve the energy efficiency and comfort of the occupants at the same time.

A Building Energy Management System (BEMS) is a computerized system that manages, monitors and controls the building services (HVAC, lighting, etc.) and energy use of buildings. It provides the information and tool that building managers can use to control the building and improve the building's overall energy

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efficiency. Control companies offer a variety of BEMS solutions, and the latest improvements in control algorithms or hardware can be implemented immediately and integrated with their own BEMS for better operational results.

For some BEMS solutions, a simulation block is embedded to provide reference data for system commissioning, fault detection and diagnostics (FDD), or simulation-based control. To ensure these functions, it is essential to perform high-quality simulation of HVAC equipment and systems in advance. Unfortunately, conventional HVAC or building simulation does not play an important role. Current HVAC models in BEMS are mainly developed by the control industry alone. Control engineers use only a highly simplified HVAC model or even a black box model in combination with system identification technology to describe the behavior of HVAC equipment.

HVAC engineers and HVAC simulation experts are ready to contribute and have made efforts to collaborate with the control industry. As shown in Table 4, several International Energy Agency (IEA) annex projects<sup>8</sup> have been conducted focusing on the use of HVAC simulation during operation and control. In practice, however, it can be seen that detailed HVAC simulation models that support the operation of the Building Energy Management System (BEMS) are still rarely used. This is a tremendous waste of major achievements in HVAC and building simulation as it simultaneously limits the benefits of simulation-based control and fault detection and diagnostic (FDD) technologies in the control industry due to the lack of accurate physical models.

### 2.4 Integral planning / Multi criteria analysis of buildings

Buildings must meet increasingly higher requirements. They must be healthy, functional, convenient and economical in everyday use, while providing flexibility for the needs of individual users, especially in commercial buildings that need to be easily adapted to changes in usage. The interior of a building must combine quality with energy efficiency, and people and assets must be adequately protected against dangers and damage. Buildings should be "green" and "intelligent". This is just a small selection of the large number of building requirements.

Theoretically, these requirements make building design a process where countless complex or even contradictory requirements must be reconciled. In the field of building practice, these subjective descriptions of requirements are expressed in quantifiable quantities that characterize the extent to which the building construction fulfills our expectations. Some common key performance indicators (KPI), such as energy consumption, cost, and PMV<sup>9</sup>, are listed in Table 5 and shown in Figure 6.

Key performance indicators make planning or operating a building a way to balance relevant valuation indices to achieve optimization. In fact, the calculation of relevant assessment indices, the optimization and balancing of several criteria such as annual energy consumption, initial costs, annual operating costs, CO<sub>2</sub> emissions, etc. are the essential aspects of building design and operation.

<sup>&</sup>lt;sup>8</sup> IEA-EBC webpage, completed projects: <u>https://iea-ebc.org/projects/completed</u>

<sup>&</sup>lt;sup>9</sup> The Predicted Mean Vote (PMV) is one of the most recognized methods of calculating thermal comfort to quantify subjective human judgment on a seven-point scale from cold (-3) to hot (+3). The PMV method according to the European Standard EN-ISO 7730 includes a specific combination of air temperature, mean radiant temperature, relative humidity, air velocity, metabolic rate, and clothing isolation.

Name	Unit	Represented objects
Annual energy consumption	W/a·m <sup>2</sup>	Energy efficiency
Initial cost	Euro	Economical factor
Annual operational cost	Euro/a·m <sup>2</sup>	Economical factor
CO <sub>2</sub> emission	kg/a	Environmental impact
PMV value	/	Human comfort
Pollutant concentration	µg/m³	Healthy





Figure 6: Multi criteria optimum balance

Obviously, building design requires a combination of different disciplines and the collaboration of many occupations: architects, civil engineers, cost estimators, HVAC engineers, mechanics, electricians and installers (MEPs), contractors and supervisors all play an important role in the building design and operation process. Good coordination and communication are of great importance when it comes to integration with such complexity. However, current coordination mechanisms in the construction industry are far from satisfactory.

In general, architects and civil engineers dominate the design and construction process. Work performed by HVAC engineers and electrical engineers is in some ways separated and treated as auxiliary tasks. It seems ridiculous to ask architects to change their design schema or work process to facilitate the work of HVAC engineers. In current construction practice, there is only a "one-way street" instead of a coordination mechanism for "mutual cooperation".

Ideally, in the design and operation of HVAC systems, energy consumption, cost, carbon footprint, and thermal comfort are key issues that need to be addressed simultaneously. In reality, however, HVAC engineers only estimate the approximate energy consumption and then select the equipment and design the detailed system according to their experience and conventions. Even for the exceptional cases in which multi-criteria analyzes have to be carried out due to the obligatory evaluation of the energy efficiency for the award of rewards, the smooth coordination and overall optimization between different domains, e.g. HVAC

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engineers, simulation experts, cost estimators and environmental impact assessment, are still rarely observed. Inseparable tasks are still isolated from each other and deliberately treated unequally.

It still seems to be an unrealistic intention to carry out a multi-criteria analysis that involves a smooth collaboration of so many fields and occupations in construction design and operations. However, the current situation does not mean that there is no internal demand for it in the construction industry. With the increasing complexity and integration of construction, increasingly complex and even conflicting requirements must be met. It is time to take concrete action to break the current inappropriate isolation and non-cooperation tradition. In reality, despite dissatisfied cooperation, designers and engineers must always at least simultaneously consider energy efficiency and initial costs, make compromises, and iteratively change design schemas to achieve the final optimal balance.

### 2.5 Multi-domain integration of building technologies

The term interdisciplinary (or multi-domain, multi-disciplinary) refers to the interaction and integration of several traditionally independent and separate disciplines. Multi-domain integration of building technologies challenges the building performance simulation to address and incorporate new emerging fields.

#### 2.5.1 Integration of renewable sources and energy storage capacities

The border line between renewable energy devices and traditional HVAC equipment is blurring. Heat and power grids are treated together as coupled systems. The modeling of user behavior is closely linked to the HVAC & Control system management. Since the development of heating systems, buildings have always acted as an energy consumer, requiring a certain amount of energy to ensure a suitable indoor climate and to use the home appliances. This consumer character has become even more pronounced following the emergence and stable supply of public utilities such as the heating, electricity and gas networks.

Today, energy policy is increasingly promoting low-carbon technologies and renewable energy sources. The decentralized generation of energy and the use of renewable energies have gained importance in recent decades. Solar thermal panels, photovoltaic (PV) panels, wind turbines and heat pumps are today commercially available devices. Local power generation devices such as photovoltaic (PV) and wind turbines offer the building designer, in addition to the use of electricity from public utility networks, another option. Building integrated photovoltaics are photovoltaic materials that are used to replace conventional building materials in parts of the building envelope such as roof, skylights or facades. The advantage of integrated photovoltaic over non-integrated systems is cost efficiency. The costs can be offset by reducing and eventually replacing the amount spent on building materials and the associated additional work (Eiffert & Kiss, 2000).

In addition to the central heat supply and the traditional fossil fuel boiler, heat could also be generated by renewable local heat generators such as solar thermal equipment, geothermal heat pumps or water heat pumps. Traditionally, HVAC engineers focus on energy consumption to maintain the desired indoor climate, and the provision of the required energy is beyond their responsibility. Accordingly, the power supply is provided by an electricity supply company, which is a matter of electricity engineers.

Similarly, the required heat of the building is supplied by a utility company. Heat generation is also not a concern of HVAC engineers. However, in combination with distributed power plants such as PV, wind turbine, heat pump, etc., the traditional consumer status of buildings is changing dramatically. Buildings switch from simple energy consumers to green electricity providers. There is an increasing demand that buildings and

communities must be considered along with the energy infrastructure when they are designed and built. Handling this revolutionary change is something that building simulation tools must address.

Electricity or heat generated from renewable (solar, wind) sources is usually sporadic and difficult to predict in nature. This intermittent generation characteristic challenges the safety and efficiency of network operation. Obviously, power storage technologies can reduce problems caused by distributed generation and increase the value of intermittent power.

Unlike other common forms of energy, such as hot water or chemical fuels such as coal, gasoline and natural gas, however, electricity must be used in their production or immediately converted into another form of energy.



Figure 7: Coupling of thermal and electrical energy

Current electricity storage methods all have their own disadvantages, as shown in Table 6. In the electricity industry, electricity storage is only achieved by transforming the form of energy. On the other hand, massive amounts of electricity are consumed on a daily basis through energy consumption devices such as HVAC systems. Electric heaters, water coolers and heat pumps consume electricity to generate heat / cold to maintain the desired indoor climate. Therefore, HVAC systems are the bridge to connect both sides, and the key to converting electrical energy into heat energy, as shown in Figure 7.

Name	Storage theory	Shortcoming
Battery	Electro-chemical	Small capacity, costly, contamination
Pumped storage	Hydro-electricity	High initial invest
Super capacitor	Electro-magnetic	Under development, classified

#### Table 6: Shortcomings of current electricity storage methods

Since great amount of electricity is consumed in building for heat or cold generation, and heat/cold storage methods are much mature: thermal energy storage can often be realized more easily and cheaply than current electrical energy storage. Building envelope, indoor air, furniture and goods inside of room, etc., all

contribute part of the overall heat capacity of building. The combined heat capacity is definitely huge. Jumbo amount of energy variation may be associated to an indoor air temperature variation of one Kelvin.

However, this enormous heat capacity of the building can only be considered as a passive energy buffer and not as an active storage. An active storage should be able to adequately store and release energy according to the instructions. Of course, it is not a false and contradictory idea to use a building as an energy store. In fact, this could only be achieved if the system technology in the building were adequately controlled.

### 2.5.2 User behavioral modeling

User behavior is absolutely one of the most important aspects of energetic considerations in buildings. Buildings and their technology can only achieve ambitious energy goals if they can be understood and properly used by building users.

However, the user is only a small part of the current building performance simulation scenario. When calculating the annual energy consumption, human actions such as switching off the air conditioner or changing the setpoint temperature are usually not well modeled. In other words, the user-supplied control signal and its control sequences are not adequately known. Instead, user behavior models are based on highly simplified hypothesis values. For example, user behavior models are still far from realistic modeling that accounts for the stochastic nature and uncertainty of typical user classes data.

Obviously, lack of importance is not the reason why the user behavior is not being adequately addressed at present. The truth is that modeling every actual user behavior in the past is extremely difficult. In early air conditioning systems, humans had no choice but to adapt the indoor climate created by the air conditioning system. Later, variable air volume (VAV) gives the local user the ability to control the local system according to their personal needs. People could control the system through a thermostat that has been placed on the wall in recent decades. However, these control actions are difficult to understand and therefore difficult to simulate.

Today mobile apps in the smartphone that can send control signals and monitor the system's operational status give people more freedom and power to conveniently and appropriately modify the operation of the building system. Currently, traditional user behavior models cannot reflect this revolutionary transformation. Future building simulations should have the ability to model cyber-physical systems in buildings. It must be possible to model and simulate every control measure initiated by the user.

The IEA-EBC Annex 66 project<sup>10</sup> was approved to address these issues. The IEA-EBC Annex 66 project aims to set up a standard occupant behavior definition platform, establish a quantitative simulation methodology to model occupant behavior in buildings, and understand the influence of occupant behavior on building energy use and the indoor environment.

### 2.5.3 Computational Fluid Dynamics (CFD)

Thermal comfort evaluation criteria such as the Predicted Mean Vote (PMV) value require three-dimensional (3D) results such as air velocity field and temperature field, which can be provided by Computational Fluid

<sup>&</sup>lt;sup>10</sup> IEA-EBC Annex 66 website: <u>https://www.annex66.org</u>

Dynamics (CFD) tools. However, CFD tools alone cannot fulfill the analysis of human comfort, they are capable predicting airflows in and around buildings, allowing a detailed assessment of building and HVAC design in terms of indoor air quality, thermal comfort and energy performance. Three-dimensional air velocity and temperature fields are subject to the immediate influence of several aspects, including: environmental conditions, HVAC system operating situation, physical adequacy of the building, etc.

Therefore, energy simulation tools and CFD tools need to be integrated in some way to meet the requirements of human comfort analysis. Energy simulation tools typically provide zero dimension results using a single average to represent the entire space, while CFD tools provide 3D fields. This means 3D and model connection issues with lower dimensions must be handled properly.



**Figure 8: Proper Orthogonal Decomposition** 

More importantly, calculating the CFD tool and processing the 3D field results is very time consuming, and energy simulation tools run much faster compared to 3D CFD tools. Roughly speaking, the calculation time of the energy simulation on the same computer usually takes several seconds, while a CFD tool takes hours or even days. This time around, disparity is a really tricky problem when two types of tools are used together. Certain interfaces and methods need to be set up to connect and coordinate the tools. The proper orthogonal decomposition method (POD) is one possible solution to this dimension / time disparity problem.

POD is a post-processing technique that is derived from detailed CFD simulations and generates reducedorder models (ROM), as shown in Figure 8. The detailed discussion of POD does not fall within the scope of this report. The reduced-order-models (ROM) generation process is a process that sacrifices some accuracy for a faster computation speed, as shown in Figure 9.



Figure 9: Balance between speed and accuracy

Using the POD method, energy simulation tools and CFD tools can be connected in a more convenient way. In addition to the study of human well-being, combined energy and CFD simulation tools could be used in many other simulation scenarios: e.g. in the design and operation of data centers and in the detailed design of HVAC systems. For example, a 3D model and a lower-dimensional model could be linked together to form

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a powerful and flexible integrated tooling system as shown in (Berger, Mazuroski, Oliveira, & Mendes, 2018; Mazuroski, Berger, Oliveira, & Mendes, 2018; Mazuroski, Oliveira, & Mendes, 2019).

# 2.6 Building life cycle integration

#### 2.6.1 Consistent information flows

The concept of the entire lifecycle is widely accepted nowadays. (Warren, 2002) suggests that an idealized process model of construction not only includes design and construction, but also commissioning, operation and renovation. The design is divided into concept design, preliminary design and detailed design. This subdivision does not mean that different life cycle stages should be isolated from each other. In contrast, it is very important that there is efficient networked collaboration between different lifecycle phases.



Figure 10: Traditional planning workflow and actual practice requirements

For example, when using data collection, some monitoring data is only stored and discarded after the completion of the monitoring project. These data are a great treasure and data mining work should be done carefully. Direct operating data such as temperature, relative humidity, CO2 concentration and energy consumption can be used in a detailed model that provides accurate performance parameters. Indirect operating data, such as effective thermal insulation values, building coverage, ventilation flow rates, heating and cooling system efficiency, could be calculated based on monitoring data to support the creation of a reduced model. Both ways would contribute to the improvement. The model that benefits from the

monitoring or data acquisition phase can provide a better design-stage result or more accurate fault detection and diagnosis (FDD) or a simulation-assisted control effect during the operational phase.

The use of lifecycle data is definitely not the only example. Early planning data can be reused for later optimization tasks. For example, the calculated net energy demand from the ideal HVAC model could later be beneficial in designing complex HVAC systems. In fact, modern building planning is an iterative and integrative process. In the early planning phase, many parameters are not yet known and preset default values based on the collected data must be used. In later planning phases, an increasing proportion of predefined default values is replaced by specific plan data. Therefore, databases must be efficiently integrated throughout the lifecycle.

In the construction practice, of course, a life-cycle-consistent information flow is required. However, as shown in Figure 10, design, simulation, commissioning, operation, and data acquisition are traditionally relatively isolated in a building lifecycle, involving multiple groups of people. Models and data are not compatible over time, and elaborate, redundant data entry is common. There is no existing generic model chain that builds the entire lifecycle to support this consistent flow of information and the demand for collaboration. The existing model chains are proprietary in-house solutions of specialized planning companies or large software companies.

In fact, the idea of a consistent flow of information across the lifecycle is very similar to the Building Information Modeling (BIM) task, but current BIM processes are highly dependent on the quality of the input data and often require manual reworking. Both building geometry and HVAC & Control systems are not adequately addressed. It is becoming more and more urgent to properly organize numerous but fragmented tools to support the construction practice from the point of view of the entire life cycle and, above all, to foster the intergroup collaboration behind it.

#### 2.6.2 Life cycle cost estimation

Designing building systems is an iterative process that has to integrate all sorts of factors simultaneously. Designers and engineers must always consider at least energy efficiency and initial cost together, compromise, and iteratively change design schemas to achieve a final optimal balance. Therefore, it makes sense to introduce the term life cycle cost simulation, which addresses the relationship between energy simulation and cost evaluation.

The total lifecycle costs (Fabrycky & Blanchard, 1991) have a major impact on the design and operation of buildings, especially in the area of contract management for building energy. The total lifecycle costs include costs for design, construction, construction, acquisition, operation, maintenance, repair, replacement and disposal.

As shown in Figure 11, the whole life cycle cost of a building can be roughly divided into three categories:

- Initial costs : purchase, acquisition, construction costs
- Operation, maintenance, and repair costs : energy costs, water costs, labor costs
- Residual values : resale or salvage values and disposal costs



#### Figure 11: Whole life cycle costs

The concept of total lifecycle costs is particularly useful when project alternatives that meet the same performance requirements, but differ in terms of initial costs and operating costs, need to be compared to select the one that maximizes the net savings and benefits. For example, total life cycle costs help determine whether the installation of a high performance HVAC or glazing system is cost effective or not. This can increase initial costs, but dramatically lower operating and maintenance costs. As life cycle analysis becomes more and more popular in recent years, cost engineers, surveyors, building economists, certified specialists, HVAC engineers, and architects use the idea of lifecycle costs to support their respective tasks. Estimating the total lifecycle cost is becoming increasingly important in the construction industry today.

The cost estimation (Wass, 1963) is an indispensable part of current construction practice, which differs significantly from building simulation, room comfort or environmental impact assessment. Construction cost estimation software is already widely used in construction practice. It is usually used by the building estimator, a person who quantifies the materials, equipment and labor required to complete a construction project and the associated costs.

Contractors usually create quotes to get a project contract on tenders. To prepare the quote, a cost estimate must first be made to determine the cost and then determine the price. During this process, the plans and specifications of the project are reviewed to generate a quantity determination. This is a list of all materials and elements required for a construction project based on construction documents. Together with the prices for these components, the quantities form the basis for calculating the direct costs. Indirect costs and profits are added together to form the final total amount. This estimated price will eventually become part of the contract.

Despite different forms of residential buildings, commercial buildings, civil engineering to activities on an urban scale, all construction projects are associated with a cost estimate. Some architects, engineers, site managers and others may also use construction cost estimation software to support their work for purposes other than bidding.

The life cycle cost calculation is based on the collaboration of the tools in two areas: building simulation and cost estimation, as shown in Figure 12. Operating cost estimation is an integral part of life cycle cost estimation. Building simulation is suitable for providing energy consumption data as basis for estimating operating costs.



Figure 12: Cooperation for life cycle cost analysis

By integrating with building simulation, a flexible and accurate lifecycle cost analysis can be achieved. In addition, dynamic simulation is the only approach to calculating energy consumption costs when integrating advanced aspects such as Demand Side Management (DSM) or local power generation equipment.

As building cost estimation software has become widely adopted and has become an indispensable tool in construction practice, life cycle cost estimation functionality associated with building cost estimation software is currently evolving rapidly. In fact, maximizing the inclusion of indispensable activities such as cost estimation is a sophisticated strategy to encourage the use of building simulations. The combination with a cost estimation tool that analyzes multiple criteria and takes initial cost, energy consumption and lifecycle costs into account together can greatly enhance the practical use of building simulation tools.

#### 2.6.3 Integrated building control and operation

Due to increasing demands, the scope and level of building control has steadily increased in recent decades. Therefore, the term building control here is a dynamically evolving and expanding definition. The building control originally came from the central plant control. Chillers and boilers were the original objects to which the control technology mainly concentrated. The invention of controlled fans or valves for a variable air volume (VAV) system has also included the control of air handling equipment and terminals. Now the control objectives are extended to the whole HVAC system.

In addition to the HVAC system, the building envelope becomes also a control target. A typical example is the recent development of climate facades (Hausladen, De Saldanha, & Liedl, 2008; Knaack & Klein, 2009; Serra, Zanghirella, & Perino, 2010), highly integrated facades with heating / cooling function. These facades themselves are a combination of envelope, HVAC equipment and control. In the case of controlled shading devices (Zawidzki, 2015), shading is carried out based on the current situation of the solar radiation, the HVAC system and the reaction of the building. There is an increasing intention to design the building envelope, the HVAC system and other related aspects together.

In traditional building planning practice, average and approximate weather information with constant facade characteristics are used to predict energy consumption. Then the HVAC engineers start with the HVAC system design based on this energy consumption data. The natural and dynamic connection between climate, building envelope, HVAC system, control strategy and building load is deliberately cut off and divided into

different parts. In the past, this separation was necessary because the possibilities of calculation were limited. But now the relationship of climate, building envelope, HVAC and their building response should be considered and controlled more carefully and in a dynamic way.

In summary, the scope of application of building control in the field of building energy has expanded considerably. An even more promising view could be obtained from the point of view of control engineers: Modern building is a combined system integrating HVAC, renewable energy devices, access and security, lighting and shading, transport (elevators / escalators), fire service, utilities, etc. In the control industry, this integrating trend is reflected in the fact that the term building energy management system (BEMS) has already been gradually upgraded to a building management system (BMS).



Figure 13: Integrated simulation application methods

So far, various integration requirements have been proposed for the development of building simulations. Now, the building simulation itself becomes an integration target, as the operation of the building system benefits from cooperation with simulation technology. There are several application methods in which simulation can support the commissioning, operation, and even software and hardware development of systems, as shown in Figure 13. To better illustrate and understand the relationship between simulation and operation, these application methods are first divided into three application relations and then presented in detail.

#### **Evaluator mode**

In the evaluator mode, the building itself and both the building equipment and the controller are codes. Simulation programs allow control engineers to test and modify designed control strategies. Various control strategies could be evaluated in advance with relatively little effort. In fact, this so-called evaluator is a conventional simulation, and HVAC engineers are better acquainted and focused on the detailed model of the building / HVAC system.

#### **Emulator mode**

In emulator mode, the building and the building equipment are virtual and are simulated. The controller is real. A typical example of an emulator is the hardware-in-the-loop technology (HiL) (Bullock, Johnson, Wells,

Kyte, & Li, 2004; Köhler, 2010, 2011; Prokhorov, 2008). HiL provides a platform on which codes are programmed instead of creating a real building system to test the functions of the controller. Simulation codes replace the real building and its HVAC systems to simulate their response to controller or building energy management system (BEMS) control commands. In addition to developing control products, emulators can also be used to train BEMS operators. Numerous operational scenarios can be generated and the BEMS operators have gained practical experience.

#### **Reality mode**

After the building and its HVAC system have been built and are present in the real world, the simulation can still contribute to the commissioning and operation of the system (Grondzik, 2009; Harmer & Henze, 2015).



Figure 14: Simulation development and its application in operation

The basic idea is to provide a reference value for control parameters in the commissioning process by simulation or to support the control decision during operation in the form of a model-predictive control (Camacho & Bordons, 2007; Ma, Kelman, Daly, & Borrelli, 2012; Wang, 2009) and a simulation-supported control (Clarke et al., 2002).

Another example is Fault Detection and Diagnosis (FDD) (Ding, 2008; Liddament, 1999), a technique that aims to detect and locate faults or to predict the presence of faults in the system. FDD uses the correct operating system model to complement the conventional feedback loop, which serves as the correct behavioral reference for the controlled system. Numerous technologies have been developed for decades to support the use of simulations on the fly, and a number of IEEE EBC Annex Energy Project projects have been completed, as illustrated in Figure 14. The use of simulations during operation will receive even more attention in the future, especially in the age of "Industry 4.0".

#### 2.6.4 "Industry 4.0" and its influence in building industry

"Industry 4.0" was originally the name for the current trend of automation and data exchange in manufacturing technologies. While the development of "Industry 4.0" is gradually increasing, it is already having an impact on the construction industry. A typical example is that the smartphone can control and monitor the operation of the building system. Of course, it's not just a transition from the thermostat on the wall to the app in the phone. The underlying cyber-physical system is to be discussed.

A cyber-physical system is a kernel foundation or even a synonym for "Industry 4.0". A Cyber-Physical System (CPS) (Geisberger & Broy, 2015; Thramboulidis, 2015) is a collaboration system of computing elements that control physical entities. The precursor generation of cyber-physical systems is often referred to as embedded systems (Hintenaus, 2016). For embedded systems, the emphasis is more on the computational elements, and for cyber-physical systems, the emphasis is more on the intensive link between computational and physical elements. A full-fledged CPS is typically designed as a network of interacting elements with physical inputs and outputs rather than standalone devices.

The idea of cyber-physics has attracted a lot of attention. Especially in the field of energy and automotive industry extensive investigations were carried out. Smart Grid and Self-Driven Cars<sup>11</sup> are representative examples of cyber-physical systems. National plans such as "Internet Plus" and "Made in China 2025" are not only "Industry 4.0" in Germany but also strategies that are strongly committed or based on cyber-physics.

In the building control industry, automated pumps or fans, flaps, etc., which could be termed actuators, are widely used in HVAC and control systems. These actuators receive a control signal from the controller to perform an action. Prior to the cyber-physical systems, there were only traditional communications between a particular actuator and its controller. One device could not communicate directly with another device. For example, in a conventional system it is not possible for a chiller to pass the sensor signal or control command directly to another chiller, but this is achieved in a cyber-physical system. In cyber-physical systems, all devices can be recognized as a communication connection point. The former control calculation is no longer the dominant function for a "CPS controller" because this control calculation function can be performed by another part of the HVAC system or even by another part of the system using cloud computing technology. The most important or even the sole responsibility for a "CPS controller" is communication. Any person or user of a building who owns a smartphone, a tablet, or a portable device can be seen as the point of communication of a cyber-physical building system. The user can directly connect and control the local VAV air terminal, chiller, flap or even central facilities. This user-centered control ensures that human comfort is actually achieved.

### 2.7 Summary of gap analysis

As buildings become more and more complex, the construction practice definitely requires integration in multiple domains, as shown in Figure 15. Although interdisciplinary approaches are increasingly being used, the situation changes only slowly. Current building simulation tools focus primarily on calculating energy

<sup>&</sup>lt;sup>11</sup> Google self-driving car project: available from <u>https://waymo.com</u>

consumption, while other influential factors affecting the economic and environmental aspects are not fully covered.



Figure 15: Multiple integration requirements

It is true that a lot of software has been developed to facilitate design, planning, operation and other building related work. However, they all focus on one or two specific areas or phases from the perspective of the entire lifecycle. This situation is completely natural and there is no reason to criticize. The real problem is that there is hardly any interflow or connection between the individual tools. The isolation between these tools, and above all the communication barriers between different domains, make building integration a real challenge.

Accordingly, models and data from different domains and stadiums are usually not compatible. It is definitely common to reenter data, which is time consuming and redundant. Although Building Information Modeling (BIM) is a widely used concept today, the current BIM focuses mainly on building data management, the integration of the entire life cycle of the HVAC and control system is just beginning, and the current coordination of architectural and HVAC-related workflows is everything others as satisfactory.

Since most simulation tools are currently too complicated and too time-consuming for designers, especially for early-stage design, "keep it simple and fast" is the general design principle of some tools<sup>12</sup>. In this case, some typical building and equipment simulation scenarios are predefined, which also work quite well. However, non-typical or non-predefined buildings or equipment, which account for most of the overall building design tasks, becomes insurmountable difficulties for these tools. In order to simulate non-typical scenarios not found in predefined cases in these tools, certain programming skills are required.

It is well known that proper requirements analysis is the very first step and foundation of software development, either from the perspective of the entire software industry. Unfortunately, many simulation tools are the results of funded projects. The requirement analyzes are therefore rather made for research reasons, which definitely leads to an application gap. To bridge this application gap, design process analyzes and associated requirements analyzes need to be used as a fundamental basis for the development and

<sup>&</sup>lt;sup>12</sup> e.g. the MIT Design Advisor: <u>http://designadvisor.mit.edu/design</u>

improvement of simulation tools to more effectively support designers and engineers (Morbitzer, Strachan, Spires, Cafferty, & Webster, 2001).

In the IEA Annex 30 project (Warren, 2002), the entire life cycle of the building is divided into several phases: design, preliminary planning, detailed planning, tender evaluation, construction and commissioning, operation and maintenance, renovation. Following this departmental definition, general objectives and typical simulation scenarios for each level can be discussed. However, simulation in current building practice is still separate from the planner or engineer's work processes. Normally, simulation experts are involved, and accordingly additional co-ordination work, additional time, and additional financial costs are inevitable, which blocks the widespread use of simulation in construction practice.

Building Information Modeling (BIM) is a typical technology designed to provide data more efficiently and to make more extensive use of data (Kensek & Noble, 2014; van Treeck & Rank, 2007). However, HVAC equipment and system simulation, which is the core component of building simulation, are not yet fully covered by currently available BIM technologies. Fortunately, it is already being observed that certain research activities are looking for suitable solutions to integrate HVAC data and models into the whole BIM community (Kohlhepp & Buchgeister, 2012; Thorade et al., 2015).

With regard to the Annex 68 project, this means that in practice, indoor air quality has so far - if at all - only been assessed using very simplified models (based on CO<sub>2</sub>). So far, the questions of indoor air quality have not found their way into dynamic building simulation. Assessments with more detailed models for the exact representation of the air flows in and around buildings are only carried out in exceptional cases. Air flow including temperature and humidity dependent pollutant sources, use of mechanistic pollutant sources in general etc. are not even established as a research area.

To sum up, simulation in construction practice is still not widespread, despite constant efforts in recent decades and research into diversity paths. According to the statements (Barbour, Rogg, Cross, & Cross, 2016) collected in the BEM workshop of 15 June 2015 (East Coast), only 20% of commercial building designs in the US use building simulation. In addition, 80% of the simulations are used merely to demonstrate compliance with the code or to obtain green building certification and are performed at the end of the design phase, which is too late to influence the designer's and owner's decision to actually take advantage the simulation advantages. There is still a long way to go to translate the simulation into practice, and much work remains to be done in the future.

Although buildings are decorated with fancy ideas such as "green" or "smart" both in research and on the market, the proportion of buildings using innovation technologies is still low when it comes to the enormous total amount of existing buildings. Energy efficiency and low-carbon technologies are mainly implemented in demonstration projects. The awareness of the urgency to translate propaganda statements into concrete measures is growing.
# **3 Building simulation integration**

# 3.1 Interdisciplinary simulation with Modelica

The demands on the simulation programs have risen massively in recent years, due to the rapid development of technology in the field of renewable energies. More and more technical components and their control algorithms have to be included in the modeling in order to achieve good quality predictions. The interaction possibilities of the models and thus the internal dependencies of the model parameters increase exponentially with their number. The core technology of the established programs is thus increasingly reaching its limits with regard to the error-free and low-maintenance maintenance of new models.

Therefore, in the field of building research from 2000 with Simulink / Modelica, a technological leap was made by importing know-how from the aerospace and automotive industries. There, the problem of the large variety of models had to be solved for a long time with a uniform simulation platform for the manufacturers of many components. The object-oriented, acausal modeling language Modelica enables domain-wide simulation of complex physical systems. This made symbolic programming possible, reducing the amount of time spent and working on a "higher level". The time-consuming development of solution algorithms could be omitted because now equations with mixed implicit / explicitly defined variables could be formulated as in a textbook. The disadvantage of this more general approach is the loss of optimization possibilities and performance on the mathematical level, for example because topological information is lost when converting into generic systems of equations.

# 3.1.1 Multi-domain modeling nature of Modelica

Modelica's multi-domain modeling makes it an ideal tool to simulate separate disciplines. The detailed vehicle model is a compelling example of such an interdisciplinary capability, as shown in Figure 16 (Otter, Elmqvist, & Mattsson, 2007).



Figure 16: Modelica multi-domain modeling

The basic idea of Modelica was to create a modeling language that could represent the behavior of models from a variety of technical fields without restricting these models to specific software. In other words, Modelica is both a modeling language and a model exchange specification. To achieve this goal, the developers of previous object-oriented modeling languages such as Allan, Dymola, NMF, ObjectMath, Omola, SIDOPS +, and Smile have been brought together with experts from many technical fields to develop the specification for the Modelica language based on their broad spectrum of experiences (Tiller, 2012).

Other features of Modelica, such as acausal, object-oriented modeling, and graphical editing, help the user focus more on describing physical behavior rather than on mathematical solution methods, as shown in Figure 17. This facilitates the acquisition of Modelica by HVAC engineers, who normally lack sound programming and math skills compared to simulation experts. Modelica is able to model an integrated building system with detailed equipment and detailed control models. Modelica models could meet the expectations of both HVAC engineers and control engineers. For example, the detailed dynamic behavior of a large thermal fluid system can be modeled by HVAC engineers while control engineers can more closely examine the control parameters.





Optimization-oriented advanced control algorithms can be conveniently simulated in Modelica. To support the building control in real time, such as: Hardware in the Loop (HiL) is a feature for which Modelica was originally developed. Modelica supports hybrid modeling, i.e. both continuous and discrete behavior can be modeled simultaneously. This feature is required to simulate digital signals and the device response of the HVAC system. Modelica is already a widely used standard language for the modeling and simulation of cyberphysical systems. In the future, Modelica could conveniently simulate human-oriented building cyber-physics systems, commands, and communications between individual objects.

# 3.1.2 Modelica building libraries

Joint efforts from research projects in an international environment, especially in Germany, have in recent years produced numerous model libraries, which in the meantime have been licensed, exchanged, linked with each other and further developed on a project-specific basis. The models are scalable to a certain degree and can be adapted to individual requirements and combined with each other. Examples are systems for the district heating supply, building simulation models, air conditioning or control engineering models. The

object-oriented Modelica technology is characterized in particular by the fact that model developers work together and libraries can be brought together as needed to a common system.

Some of the Modelica based building/system libraries are listed in Table 7. The goal here is not to show the exact number of organizations involved and published documents, but the list of existing libraries and models gives the general impression that current Modelica libraries and models are already the most commonly used in the HVAC and Control field.

Library name	Author organization
MSL.Fluid, MSL.Thermal <sup>13</sup>	Modelica Association
BuildingSystems <sup>14</sup>	Berlin University of the Arts
Buildings <sup>15</sup>	Lawrence Berkeley National Laboratory
ATplus v2.1 (Merz, 2002)	Institute of Automatic Control, TU Kaiserslautern
Green Building <sup>16</sup>	EA Systems Dresden GmbH
AixLib (Fuchs et al., 2015)	RWTH Aachen University
IDEAS (Baetens et al., 2015)	KU Leuven
RECOMB (Hoffmann & Kahler, 2003)	TU Ilmenau and De Montfort University
HITLib (Videla & Lie, 2006)	Telemark University College
BuildSysPro (Plessis, Kaemmerlen, & Lindsay, 2014)	EDF R&D EnerBat
IDA ICE17	EQUA Simulation AB
TechThermo (Steinmann & Zunft, 2002)	DLR (German Aerospace Center)
ThermoPower <sup>18</sup>	Informazione Politecnico di Milano

## Table 7: Existing Modelica based building libraries

There are also many organizations around the world who contribute to the development of Modelica models in a non-library way. Some of them are listed below:

- Fraunhofer Institute for Solar Energy Systems (Burhenne, Wystrcil, Elci, Narmsara, & Herkel, 2013)
- Fraunhofer Institute for Building Physics (Pathak, Norrefeldt, Lemouedda, & Grün, 2014)
- Hermann-Rietschel Institute, TU Berlin (Hoh, Haase, Tschirner, & Müller, 2005)
- Department of Technical Thermodynamics, TU Hamburg-Harburg (Wischhusen, Lüdemann, & Schmitz, 2003)

<sup>&</sup>lt;sup>13</sup> Homepage of the modelica association: <u>https://www.modelica.org</u>

<sup>&</sup>lt;sup>14</sup> Homepage building systems modelica library: <u>http://modelica-buildingsystems.de</u>

<sup>&</sup>lt;sup>15</sup> Homepage buildings modelica library: <u>https://simulationresearch.lbl.gov/modelica</u>

<sup>&</sup>lt;sup>16</sup> Green building website: <u>http://www.eaenergie.de/en/products/green-building-simulationsbibliothek-2-2</u>

<sup>&</sup>lt;sup>17</sup> Ida indoor climate and energy website: <u>https://www.equa.se/en</u>

<sup>&</sup>lt;sup>18</sup> ThermoPower repository: <u>https://github.com/casella/ThermoPower</u>

- Swiss Federal Institute of Technology Zurich (ETH) (Fabricius & Badreddin, 2002)
- Department of Mechanical Engineering, University of Wisconsin (Li, Li, & Seem, 2008, 2010)
- Department of Automatic Control, Lund Institute of Technology (Eborn, 2001; Tummescheit, Eborn, & Wagner, 2000)
- Institute for Thermodynamics, TU Braunschweig (Junior, Strupp, Lemke, & Köhler, 2009)

The rapid development since 2000, however, led to different, sometimes incompatible Modelica libraries for modeling and simulation of building energy supply systems and the control technology. The diversification process was favored by various development environments<sup>19</sup>.

A representative of the libraries is the freely available Modelica Buildings library, which was developed at the Lawrence Berkeley National Laboratory in the USA. It includes component models for the simulation of building energy systems and controls based on the Modelica Fluid Library, a library for the simulation of the behavior of hydraulic systems. Particular attention is paid to the detailed illustration of heating, ventilation and air conditioning systems.

A comparable library was developed at the E.ON Energy Research Center of the RWTH Aachen, the Modelica Building Library AixLib. This includes detailed components for mapping thermal building behavior as well as comprehensive models of heating, ventilation and air conditioning technology. In addition, it contains a comprehensive database of building physical material values as well as manufacturer information for the parameterization of plant components.

The Modelica BuildingSystems library was also developed in Germany, at the Chair of Supply Planning, Supply Engineering Institute of Architecture and Urban Design of the UdK Berlin. The components include a broad spectrum from the areas of space and buildings, solar energy technology (photovoltaics and solar thermal energy) as well as heating and air conditioning technology. The focus of library is on the modeling and simulation of heat distribution systems. Therefore, there are a variety of system components in different spatial or physical depth of detail, for example, the construction of a local heating network model or the detailed model of the hydraulic network of a heating system.

Other building simulation libraries include the open-source OpenIDEAS library of KU Leuven from Belgium, as well as the non-open BuildingPhysics library of the Fraunhofer Institute for Building Physics, which was developed for thermal and hygrothermal building simulation. Another area of application covers the Human Comfort Library of XRG Simulation GmbH. This library provides models for calculating, simulating, and predicting the comfort of people with thermal comfort in air-conditioned rooms. It can be used in combination with other Modelica-based libraries that enable simulation of air conditioning and heating systems as well as complex building zone behavior.

The Green Building Library distributed by ITI GmbH was developed as part of a research project by EASD EnergieArchitektur GmbH and the Institute of Automotive Engineering Dresden (IAD). The aim was to develop a test platform for the development of new energy management systems for regeneratively supplied buildings, which allows the connection, the test and the validation of the designed algorithms on a as detailed

<sup>&</sup>lt;sup>19</sup> Modelica development environments include i.a. SimulationX of ITI GmbH, Dymola of Dassault Systèmes and MapleSim of MapleSoft

as possible simulated building energy system. The library's main focus is on the electrical and thermal components, the regenerative building energy systems and the storage facilities (including vehicles with electrified powertrain and external charging interface) as well as their interaction.

In the conclusion, Modelica can be used by specialized teams of experts, which limits the use of libraries in the broader context. However, Modelica Model Libraries are well suited to be plugged into other simulation environments to extend them.

# 3.1.3 Annex 60 cooperative buildings library development

In 2017, together with the IEA EBC Annex 60 Final Report, the Modelica Annex 60 Library was published as part of the Energy in Buildings and Communities (EBC) program of the International Energy Agency (IEA) "Computer-Aided Tools for Buildings and Municipal Energy Systems". The Modelica Annex 60 library will now be further developed within the framework of the IBPSA project 1<sup>20</sup>. It is an international effort to build a unified Modelica Library for building simulation.

As shown in Figure 18, four major contributors, the Lawrence Berkeley National Laboratory, the RWTH Aachen, the Berlin University of the Arts, the KU Leuven, and other associated organizations are working together to develop this Modelica Annex 60 library. The contributors of the Modelica Annex 60 Library have already created four known Modelica libraries individually: BuildingSystems, Buildings, AixLib, IDEAS.



Figure 18: Integration of Modelica libraries

The Modelica Annex 60 Library provides reliable base classes for building and HVAC component models. Developers of the various model libraries then integrate base classes into their library, add additional models, provide documentation and user support. Through this process, the different libraries with different emphases can be further developed while ensuring compatibility. Compared to the previously fragmented development of incompatible libraries, a reliable and proven common foundation for model development is

<sup>&</sup>lt;sup>20</sup> IBPSA Project 1 "BIM/GIS and Modelica Framework for building and community energy system design and operation": <u>https://ibpsa.github.io/project1</u>

certainly a clear advantage. The Modelica Annex 60 Library is not just a simple link between these four existing Modelica libraries, it's a new achievement with extensive collaboration.

To automatically merge the Modelica Annex 60 Library with libraries based on it, such as the latest version of AixLib, Buildings, BuildingSystems, and IDEAS, developers of these libraries can use a BuildingsPy Python package. BuildingsPy can update all hyperlinks, package name references, and filenames that contain the Annex60 string. Therefore, users only see the library and do not need to combine models from different libraries. In other words, the Modelica Annex 60 Library includes hundreds of sub-models for energy building and facility simulation managed through a common development platform. This consistent and freely available approach solves the problem of incompatibilities and inadequate interchangeability between the previously separate libraries and makes the library openly accessible through an open source model.

The establishment of this Annex 60 library is a great impetus to the application of Modelica based building simulation. Numerous unified and high quality models are provided along with this library, which definitely is a valuable resource for further practical usage in both design and operation activities. At the end, one paragraph quoted from Annex 60 final report is directly written here as closure of this chapter, since this statement given by cooperative development participants themselves is the most appropriate commentary for Annex for 60 library and all cooperative development activities.

The development of the Modelica Annex 60 Library will provide an important impetus for the use of Modelicabased building simulation. Together with this library, numerous high quality models are provided. This is definitely a valuable resource for further practical use in both planning and operational activities. At the end of this chapter, a paragraph from Annex 60 of the Final Report is cited directly, as this statement is the most appropriate commentary on co-operative development activities within the Annex 60 itself.

"At the first expert meeting of the planning phase of Annex 60, in March 2013 at RWTH Aachen, Germany, participants were hesitant to open up their proprietary development, open-source their code and embark on a joint development of an open-source library that should become the core of their respective libraries. However, as the collaborations slowly took shape, participants saw the value in avoiding duplicative work, in conducting collaborative research and in jointly developing a core library. Hence, participants ended up investing a considerable amount of work in scrutinizing different implementations, refactoring their respective libraries for building and district energy systems now all share the same set of core models, they became more robust, better validated and compatible with each other. With this shared development, Annex 60 created a robust, open-source basis for a model library for the buildings performance simulation community."<sup>21</sup>

# 3.2 CHAMPS collaboration platform approach

New technologies such as Modelica alone are not enough to coordinate the workflow in practice and to support simulation integration in the construction industry. They provide support at the technological level, but such technologies are rarely used, especially in early planning stages. Further efforts are needed to advance integrated planning in practice using simulation tools.

<sup>&</sup>lt;sup>21</sup> Statement from the Co-Operating Agent of the IEA-EBC Annex 60 project, Christoph van Treeck, 2017

# 3.2.1 Introduction to the CHAMPS modeling platform

As part of the work under subtask 3 of Annex 68, a CHAMPS modeling platform (Figure 19) was set up. The focus of this multiscale and multidisciplinary modeling platform is on integration and use of free solvers developed in the scientific community. These solvers deal with building processes related to air, light, energy, HVAC operation, moisture and pollutants.



Figure 19: Multi-scale and multi-disciplinary CHAMPS modeling platform

The simulations can be setup using the graphical user interface BIM HVAC Tool<sup>22</sup>, jointly developed by Tian Building Engineering and the TU Dresden, Institute of Building Climatology, which greatly facilitates pre- and post-processing. While all solvers are free programs, is the BIM HVAC Tool the only commercially distributed software on the CHAMPS modeling platform.

The available free solvers on the CHAMPS-platform are:

OpenFOAM<sup>23</sup> is the free, open source CFD software developed primarily by OpenCFD Ltd since 2004. It
has a large user base across most areas of engineering and science, from both commercial and academic
organizations. OpenFOAM has an extensive range of features to solve anything from complex fluid flows
involving chemical reactions, turbulence and heat transfer, to acoustics, solid mechanics and
electromagnetics. OpenFOAM is professionally released every six months to include customer sponsored
developments and contributions from the community. It is independently tested by ESI-OpenCFD's

<sup>&</sup>lt;sup>22</sup> https://building-engineering.de/

<sup>&</sup>lt;sup>23</sup> https://openfoam.com/

Application Specialists, Development Partners and selected customers, and supported by ESI's worldwide infrastructure, values and commitment.

- Radiance software<sup>24</sup> is a distributed raytracing package developed by Greg Ward Larson, then at the Lawrence Berkeley National Laboratory (LBNL) in Berkeley, California. Radiance is currently the most powerful and robust system for computing the effects of architectural lighting and *daylighting*, and can output images in photorealistic (or rather "photo accurate", as its author claims) quality. Consequently, the special image format used does not store subjective "brightness" values, but the actual *luminance* on all visible surfaces. Apart from that, Radiance can compute *illuminance* values at arbitrary points in space, which is useful to determine *daylight factors* and illuminance levels on the *workplane*.
- NANDRAD<sup>25</sup> is a modern building energy simulation platform for the dynamic analysis of the energy efficiency of a building. It is actively developed at the TU Dresden, Institute of Building Climatology especially for calculation of complex and large buildings, and to handle the large amount of data for such building sizes. At the same time, the integrated physical models are quite detailed, which is meaningful for a dynamic description of the building behavior. In particular, massive construction form in the European area are well represented by spatially discretized constructions.

The resulting physical models place high demands on the numerical integration engine. Hence, the NANDRAD solver was specifically developed and optimized for building energy simulation, and uses stateof-the-art technology in embedded numerical algorithms.

Besides intern equipment and control models, NANDRAD supports runtime simulation coupling based on the Functional Mock-up Interface (FMI), Standard 2.0. Through this it is possible, to combine detailed equipment/HVAC system models and components, mostly on the supply side, from specialized simulation tools/libraries (e.g. Modelica) with the NANDRAD building energy simulation.

- DELPHIN<sup>26</sup> is a comprehensive numerical simulation tool for the combined heat, air, moisture, and matter (e.g. salt) transport in porous building materials. DELPHIN supports runtime simulation coupling based on the Functional Mock-up Interface (FMI), Standard 2.0. For further information, see subsection 3.3.3 "Co-Simulation with DELPHIN6". DELPHIN is actively developed at the TU Dresden, Institute of Building Climatology.
- EnergyPlus<sup>™27</sup> is the reference program for NANDRAD on the CHAMPS platform. It is a whole building energy simulation program that engineers, architects, and researchers use to model both energy consumption for heating, cooling, ventilation, lighting and plug and process loads and water use in buildings. EnergyPlus is a console-based program that reads input and writes output to text files. It ships with a number of utilities including IDF-Editor for creating input files using a simple spreadsheet-like interface, EP-Launch for managing input and output files and performing batch simulations, and EP-Compare for graphically comparing the results of two or more simulations.

<sup>&</sup>lt;sup>24</sup> https://windows.lbl.gov/software/radiance

<sup>&</sup>lt;sup>25</sup> https://bauklimatik-dresden.de/nandrad/index.php

<sup>&</sup>lt;sup>26</sup> https://bauklimatik-dresden.de/delphin/index.php

<sup>&</sup>lt;sup>27</sup> https://energyplus.net/

- **Modelica Annex 60 Library**<sup>28</sup> is a free library that provides basic classes for the development of Modelica libraries for building and community energy and control systems. The intent of the library is that classes of this library will be extended by implementations of Modelica libraries that are targeted to end-users. Hence, this library is typically not used directly by end-users, but rather by developers of libraries that will be distributed to end-users. For more information, see subsection 3.1.3 "Annex 60 cooperative buildings library development".
- MASTERSIM<sup>29</sup> is an FMI Co-Simulation master and programming library. It supports the Functional Mockup Interface for Co-Simulation in Version 1.0 and 2.0. Using the functionality of Version 2.0, it implements various iteration algorithms that rollback Functional Mock-up Unit (FMU) slaves and increase stability of coupled simulation. MASTERSIM is actively developed at the TU Dresden, Institute of Building Climatology. The MASTERSIM installers are being hosted on SourceForge.
- POSTPROC<sup>30</sup> The scientific post-processing software was developed specifically for analyzing simulation results of our software DELPHIN, THERAKLES, NANDRAD and MASTERSIM, primarily focusing on timedependent/dynamic data. However, due to its flexible data interface, it can be used for many other purposes like processing of measurement data and results of other simulation models. POSTPROC is actively developed at the TU Dresden, Institute of Building Climatology.

During the course of the Annex 68 project, the developmental work focused on implementation of diffusion and emission of pollutants in DELPHIN6. Another important aspect was the development of coupling technologies to support co-simulation. Finally, an extensive gap analysis and two common exercises revealed further implementation demand and the necessity of quality assurance management. In the following sections, several application examples demonstrate the broad range of topics and scenarios that can already be addressed by using single or coupled tools from the CHAMPS modeling platform.

# 3.2.2 CHAMPS application example 1: University Campus TU Dresden

A first application example of the CHAMPS simulation platform comes from a so-called EnEff-Campus project for energy analysis (tools used are Radiance, EnergyPlus, NANDRAD, DELPHIN, POSTPROC). As can be seen in Figure 20 on the front page, the Campus of the Dresden University of Technology serves as a study object.

The overall objective of the project was to draw up an energy development plan with short-, medium- and long-term measures to reduce energy consumption on the campus. These included the development of an optimized energy supply strategy, taking into account the urban context, the scientific monitoring of practical reconstruction measures and the testing of innovative energy management systems. On the basis of a detailed analysis of the current status, a development concept for the energy supply of the campus and the energetic upgrading of the buildings as well as their networking regarding the heating and cooling supply was developed.

To this end, full-scale building models have been created on the basis of existing CAD plans. One research question was to examine the sensitivity of the simulated energy consumption (heating energy vs. electricity) as a function of the level of detail (e.g. number of modeled / merged zones). One lesson learned was that in

<sup>&</sup>lt;sup>28</sup> http://www.iea-annex60.org/news.html#modelica-annex-60-library-released

<sup>&</sup>lt;sup>29</sup> https://bauklimatik-dresden.de/mastersim/index.php?aLa=en

<sup>&</sup>lt;sup>30</sup> https://bauklimatik-dresden.de/postproc/index.php

office buildings a minimum level of detail must be maintained in order to keep the ratio of heating energy to electricity within a realistic range. Due to the increased lighting demand in merged zones, the power consumption can be overestimated and the heating energy underestimated if the level of detail is too low.



Figure 20: Simulation models of selected buildings on the TU Dresden Campus

# 3.2.3 CHAMPS application example 2: Whole building energy analysis in the City of Geretsried

A second application example shows the achieved progress of the platform in the area of practice integration (tools used are Radiance, EnergyPlus, NANDRAD, POSTPROC). In the frame of the research project +EQ-Net, a residential area in the city center of Geretsried in Germany was examined (Figure 21).



Figure 21: Simulation model of a residential and commercial building in the City of Geretsried, Germany

Energy concepts were developed by means of variant studies / scenarios that evaluated the energetic selfsufficiency and grid compatibility of the whole building. The framework conditions of the pilot project were:

- Planned new building for multi families with additional commercial units
- Variant study in the early planning phase
- Energy concept for self-sufficient supply of heat and electricity

• Creation of a certificate for a positive energy balance throughout the year

During the project, models with varying degree of detail were created. Simplified models in the beginning of the project phase contained combined zones. However, these models are conditionally suitable for a study of thermal comfort since mathematically averaged values, over a large area of merged zones, have little or no significance. Therefore, refined models with more detailed representations of thermal zones have emerged. Furthermore, the designs have been adapted or changed according to the progress in the planning process. It could be shown that tools from the CHAMPS modeling platform can already be successfully used in practice and can keep pace with planning progress.

# 3.2.4 CHAMPS application example 3: Coupled plant and single zone model

The third application example demonstrates newly developed technology in coupling of building and plant models (Figure 22) that supports integral planning including very different domains in the field of building performance simulation. One important topic was the development of a largely automated and script-supported workflow that addresses creation of so-called Functional Mock-up Units (FMUs) according to the Functional Mock-up Interface (FMI) standard and the definition of coupling scenarios.



Figure 22: Co-simulation of a plant model and a building model by using Modelica and NANDRAD

The application of co-simulation technology will only be effective in practice and in the academic environment if the effort for the definition and implementation, including the evaluation, remains within a reasonable and economically justifiable frame. This includes also the time spent on troubleshooting. A reduction of this processing effort is strongly linked to the respective procedure and the question to be worked on, the development of an adapters and wrapper technology. Adapters and wrapper-Models significantly simplify connecting FMUs with hundreds of input/output variables.

For the efficient use of the coupling technology, the FMU import procedure had to be improved. The idea was that FMU and connector models (*AmbientConditions-Adapters*) would be wrapped together in a Modelica

model. The wrapper models are Modelica models, so they can easily be generated automatically via script or as part of the export.

With NANDRAD, the number of interfaces depends on the building model, specifically the number of zones and the respective zone IDs, so that the wrapper must be created appropriately for each FMU export. To automate this, the generated Modelica source code was analyzed and a template for automatic replacement of the FMU-specific connectors was created. The NANDRAD FMU export source code has now been extended to fill this template project specific. This allows the wrapper to be created automatically with the FMU, simplifying the import procedure and linking.

# 3.2.5 CHAMPS application example 4: Soil heat collector simulation

The fourth application example demonstrates the use of the CHAMPS modeling platform in simulation of renewable heat sources (Figure 23). The simulation of the hygrothermal behavior of the ground including ice formation makes it possible to describe very precisely and to optimize the operation of ground heat exchangers installed in a depth of 2-5 m. At the surface, the data from the test reference year (TRY) of the German Weather Service is used that includes temperature, relative humidity, direct radiation, diffuse radiation, atmospheric counter radiation and hourly precipitation for a representative year. The average terrestrial heat flux from the earth's interior can also be taken into account.

Starting from an undisturbed earth temperature field (no operation in the first year of the simulation), the courses of the ground temperatures in selected positions are evaluated in the following nine years of operation. The moisture content of the soil is an important factor that contributes significantly to the functioning of the system. The water in the soil itself has a high heat storage capacity and the periodic ice formation contributes to the amount of heating and cooling energy that can be delivered from the ground source. If underground ice is formed by harvesting more heating energy in wintertime, additional cooling energy can be provided in summer, which supports the regeneration of the collector fields and provides a bidirectional seasonal shift of energy.





Figure 23: Single soil heat collector (middle) that can be combined to collector fields (right)



Figure 24: Temperature and ice field of the soil calculation domain (20 x 25 m) with one embedded collector field

This requires coupling of DELPHIN6 for high performance simulation of large problems with the Modelica AixLib<sup>31</sup> for dynamic simulation of district networks. Both programs must support the FMI standard 2.0. In addition, the development of the simulation master MASTERSIM<sup>32</sup> was necessary that coordinates the run of the co-simulation.

# 3.3 Integration through the Functional Mock-up Interface

Functional Mock-up Interface (FMI) is a tool independent standard to support both model exchange and cosimulation of dynamic models using a combination of xml-files and compiled C-code<sup>33</sup>. The first version, FMI 1.0, was published in 2010, followed by FMI 2.0 in July 2014. The FMI development was initiated by Daimler AG with the goal to improve the exchange of simulation models between suppliers and OEMs. As of today, development of the standard continues through the participation of 16 companies and research institutes under the roof of the Modelica Association as a Modelica Association Project. FMI is supported by over 100 tools and is used by automotive and non-automotive organizations throughout Europe, Asia and North America.

# 3.3.1 Application of the FMI standard in the building sector

In order to achieve an integration between the tools, the coupling of different simulators is necessary. Building simulation tools can be linked together to make workflow collaboration more efficient. In a coordinated network environment, tool interoperability is paramount and needs to be carefully developed. Obviously, international regulations and generally accepted standards such as FMI are a necessary precondition for interoperability. Once interoperability is assured, models or tools are created according to

<sup>&</sup>lt;sup>31</sup> AixLib isa Modelica model library for creating building and system simulations. The library is being developed at the E.ON Energy Research Center, Chair for Building and Indoor Climate Technology at RWTH Aachen University. Download link: http://ibpsagermany.org/wordpress/tools

<sup>&</sup>lt;sup>32</sup> MASTERSIM is a free tool to coordinate co-simulation. Download link: http://ibpsa-germany.org/wordpress/tools

<sup>&</sup>lt;sup>33</sup> Homepage of the FMI standard: <u>https://fmi-standard.org</u>

the same protocol, and these models and tools can be more conveniently integrated in design and construction practice.

There are several methods to implement a simulation connection. So far, the main connection method is a one-to-one connection that is created individually. For example, Simulink models are linked to Modelica models using Simelica and the AdvancedBlocks library (Dempsey, 2003). The coupling between CFD and thermal computation is achieved using the Boltzmann discrete-speed equation (Brown, Augenbroe, Choudhary, & Paredis, 2009). The Matlab Advanced Control Model is combined with Modelica models and then simulated with the HQP solver (Hoffmann & Puta, 2006).

The model / tool coupling functionality can then also be implemented via middleware provided by a third party. TISC (Kossel, Tegethoff, Bodmann, & Lemke, 2006; Ljubijankic, Nytsch-Geusen, Rädler, & Löffler, 2011), COSimA+ (Stratbücker, van Treeck, Bolineni, Wölki, & Holm, 2011), Virtual Test Bed (BCVTB) for Building Control (Wetter, 2011; Wetter & Haves, 2008) connect models and tools from different sources and demonstrate a competitive optional integration path. As models are affected by many different resources, appropriate standards and protocols must be developed to ensure interoperability during the tool integration process. Therefore, the FMI standard (Functional Mock-up Interface) has been created to connect models or tools in a standardized way.

The Functional Mock-up Interface (FMI) standard defines a runtime interface for the data exchange of coupled, dynamic simulation programs. In addition, the content and the format of a description file are defined, as well as a directory structure for the data to be exchanged. By standardizing formerly proprietary interfaces, it is now possible to couple simulation models from a wide variety of simulation environments.

There are two modes of operation:

- FMI for ModelExchange: A central ModelExchange master completes a coupled time integration of the differential equations of all coupled FMUs. Since simulation programs (such as DELPHIN6) result in a large number of coupled differential equations, the respective model-specific structure must be included in the solution procedure for efficient time integration (specifically, the support of sparse Jacobian matrices). A generic ModelExchange master program without this knowledge of the system almost inevitably has a (much) worse performance. The use of ModelExchange is therefore not expedient for applications with a large number of coupled differential equations.
- FMI for CoSimulation: Each simulation model works in a similar way to a self-functioning simulation model and has its own time integrator. In contrast to the standalone version, the simulation is interrupted after a communication interval and the Co-simulation master can exchange data between FMUs. Interrupting the simulation and selectively updating the input variables results in some overhead depending on the time integration algorithm, but within each FMU, the respective optimal time integration method can be implemented.

# 3.3.2 Development of MASTERSIM in the EnTool:CoSim project



The development of the MASTERSIM program<sup>34</sup> is an outcome of the EnTool:CoSim project, a collaborative research project financially funded by the German Federal Ministry for Economic Affairs and Energy under file number BMWi 02E23S6205. Participating partners were: Dresden University of Technology, ITI GmbH, Fraunhofer Institute for Integrated Circuits and EA Systems Dresden GmbH. In EnTool:CoSim,

concepts and methods for the efficient coupling of runtime-optimized building models with Modelica-based plant models were developed in order to combine the advantages of both modeling approaches.

The technology is based on the already standardized Functional Mock-up Interface for co-simulation. The challenges are the building model size and the very different numerical properties of the model components. Particular attention is paid to the optimization of the overall calculation speed, the problem-oriented evaluation of results, as well as the usability of the procedures in practice.

MASTERSIM is an open-source co-simulation master implementation that supports FMI 1.0 and 2.0. The master employs several algorithms for obtaining stable, efficient and error controlled solutions. It contains:

- Different master algorithms/iteration methods, such as non-iterative Gauss-Jacobi, and iterative Gauss-Seidel and Newton methods,
- Variable communication step sizes with local error control,
- Serialization/deserialization for stop-and-restart of the master.

MASTERSIM is developed in C++ and runs on Windows, Mac OS X and Linux. Also, the master supports a feature that disables automatic unzipping of FMU archives, which allows for using persistent DLL/shared library files, which is important for FMU developers. MASTERSIM is available from http://mastersim.sourceforge.net under a GPL v3.0 license.

Special features of MASTERSIM are:

- Scripting possibilities: MASTERSIM can be used from scripts, for example when variation studies are done. For that purpose, project files are plain-text and can created/edited with scripts easily. The actual simulator is provided as command line executable MasterSimulator, which can be called from scripts.
- Assisting FMU Development: MASTERSIM can be configured via command line arguments to extract FMUs automatically, or use already extracted FMUs. This allows compilation of the shared libraries/DLLs in debug mode and let MASTERSIM load these libraries, instead of those packaged in the FMU, which allows external debugger use. Also, you can directly fix errors in the model description file without unpacking/repacking the FMU archive.
- Simulation Scenarios with several FMU instances: MasterSim supports multiple instances of the same FMU within one simulation scenario. In order to avoid FMU instances overwriting each other's results, a directory structure layout is defined and FMU-specific base paths are communicated to each FMU slave. This allows batch processing/parallel execution of several simulation scenarios (runs of MasterSimulator) where the same FMU is instantiated many times.

<sup>&</sup>lt;sup>34</sup> A reference to MASTERSIM can be found at: <u>http://ibpsa-germany.org/wordpress/tools</u>

The following scientific publications, research and technical reports are available about MASTERSIM:

- Nicolai, A.; Co-Simulations-Masteralgorithmen Analyse und Details der Implementierung am Beispiel des Masterprogramms MASTERSIM, 2018<sup>35</sup>
- Nicolai, A.; Co-Simulation-Test Case: Predator-Prey (Lotka-Volterra) System, 2018, Technical Report<sup>36</sup>
- Nicolai, A. and Paepcke, A.; *Co-Simulation between detailed building energy performance simulation and Modelica HVAC component models*, 2017, 12th International Modelica Conference, Prague<sup>37</sup>
- Nicolai, A., Paepcke, A. and Hirsch, H.; *Robust and accurate co-simulation master algorithms applied to FMI slaves with discontinuous signals using FMI 2.0 features*, 2019, 13th International Modelica Conference, Munich<sup>38</sup>
- Nicolai, A.; Validierung des Co-Simulations-Masterprogramms MASTERSIM, 2019, Technical Report<sup>39</sup>

# 3.3.3 Co-Simulation with DELPHIN6



DELPHIN<sup>40</sup> is a simulation program for the coupled heat, moisture, and matter transport in porous building materials. During the course of the Annex 68 project, it has been equipped with a FMI-interface for Co-Simulation. The DELPHIN software is used for a range of different engineering applications:

- Calculation of thermal bridges including evaluation of hygrothermal problem areas (surface condensation, interstitial condensation)
- Design and evaluation of inside insulation systems
- Evaluation of ventilated facade systems, ventilated roofs
- Transient calculation of annual heating energy demand (under consideration of moisture dependent thermal conductivity)
- Drying problems (basements, construction moisture, flood, ...)
- Calculation of mold growth risks
- ... and further applications

DELPHIN is used in research and development for:

- Material development and optimization
- Research of salt transport and salt related damage and degradation of building materials
- Description of pollutant/VOC transport (emission) in multi-layered constructions and materials
- Simulation of hygrothermal behavior of the soil with ground heat exchangers (geothermal collectors)
- ... and several other research areas

<sup>&</sup>lt;sup>35</sup> Access via Qucosa: <u>http://nbn-resolving.de/urn:nbn:de:bsz:14-qucosa2-319735</u>, Full text pdf version available under: <u>Nicolai\_MasterSim\_Algorithmus.pdf</u>

<sup>&</sup>lt;sup>36</sup> Full text pdf version available under: <u>Nicolai MasterSim ErrorTests with Lotka Volterra Model.pdf</u>

<sup>&</sup>lt;sup>37</sup> Full text pdf version available under: <u>Nicolai Modelica NANDRAD CoSim 2017.pdf</u>

<sup>&</sup>lt;sup>38</sup> Full text pdf version available under: <u>Nicolai\_et\_al\_2019\_ModelicaConference.pdf</u>

<sup>&</sup>lt;sup>39</sup> Full text pdf version available under: <u>Nicolai Validierung des CoSimulations Masterprogramms MasterSim.pdf</u>

<sup>&</sup>lt;sup>40</sup> A reference to DELPHIN can be found at: <u>https://bauklimatik-dresden.de</u>



Figure 25: Hygrothermal Simulation of a roof construction with DELPHIN

For a number of applications it is necessary to couple DELPHIN with other simulators. This concerns e.g. the simulation of buildings with geometrically complex building parts that cannot be idealized as 2D objects. The coupling of geothermal collectors with a district heating network also requires model-side coupling. To perform a co-simulation with DELPHIN, the following procedure is provided:

- 1. Defining / adapting the DELPHIN model and, if necessary, single calculation with constant / predefined input variables
- 2. Define the input variables and output variables
- 3. Exporting the FMU (if necessary, updating an existing FMU)
- 4. Opening a co-simulation master (e.g. MASTERSIM)
- 5. Configure the simulation scenario / link the variables
- 6. Perform and analyze the simulation

For changes to the DELPHIN model, steps 1-3 should be repeated.

## Input variables

All input variables, which are later transferred to the FMU from the master program, are in the DELPHIN climate conditions. Climate conditions can be used as time series in boundary conditions and source / sink models. In order for FMU Export to define an environmental condition as an input variable, the type (time history) in the climate condition dialog must be set to *Generated by external model (FMI) [External]* (Figure 26).

Climate condition	×
Specification	
Name: New climate condition	
Type: Mass flow rate [MassFlowRate]	V Kind: Generated by external model (FMI) [External]
FMU Import Options	
Variable name/reference: Climate	Cond.New_climate_condition
Default value (when input is not connected):	kg/s
Note: The default value is only used, when there is no given in the unit shown above!	input connected to the DELPHIN FMU. If the Co-Simulation master provides an input value to the DELPHIN FMU for this variable, it is expected to be

Figure 26: Climate condition dialog - definition of an FMI input variable. The FMI variable name always has the form *ClimateCond.<Name>* and the unit is given according to the physical size.

Any climate condition defined with *Type = External* will later appear as an interface variable in the FMU, but only if the climate condition is also used somewhere. The physical unit is fixed for each physical variable and cannot be changed during export. Accordingly, when linking different FMUs, attention must be paid to correct units and, if necessary, the unit be converted into an FMU.

The FMI variable name always consists of the name of the climate condition and the prefix "ClimateCond.".

**Default values for input variables:** Each FMI input variable must have a default value which is used when no value is given by the co-simulation master, i.e. if this variable was not linked to output variables of other FMUs. The unit of this parameter is defined in the climate condition dialog depending on the physical size and thus defines the unit of the variable which is transferred to the FMU. In the example in Figure 26, the input variable is expected in degrees Celsius.

## **Output variables / results**

FMU result variables are generated automatically, according to the following rules:

- For each output file that yields a scalar value, an output variable of the same name is created automatically. Scalar outputs are obtained, for example, at sensor values, i.e. output quantities selected on a coordinate or in a single cell, or of space integrals /averages.
- In addition, certain models generate additional scalar result quantities that are not directly assigned. An example of this is the pipe collector model: boundary condition *heat conduction*, type *heat transfer from pipe with flowing fluid [PipeCollectorModel]*. With the definition of this boundary condition, these additional results can be activated (see Figure 27). These results also appear as output variables of the FMU.

Boundary condition			>			
Specification						
Name: Heat condu	tion boundary condition					
Type: Heat condu	e: Heat conduction [HeatConduction] $\vee$ Kind: Heat transfer from pipe with flowing fluid in a material [PipeCollectorModel] $\vee$					
Schedule: <pre></pre>	ie/always enabled>	~ C	reate new			
Climate data						
Temperature	[Current location]::Temperature	~ 0	reate new			
Imposed heat flux	<select create="" new="" or=""></select>	✓ 0	reate new			
Wind velocity	<select create="" new="" or=""></select>	~ c	reate new			
Mass flow rate	Mass flux	~	Edit			
Heat transfer coefficier	t <select create="" new="" or=""></select>	~ C	reate new			
Heat load/power	<select create="" new="" or=""></select>	✓ 0	reate new			
Parameter Specify pipe collecto	or inlet temperature					
Exchange coefficient fo	r still air [W/m2K]:		12			
Slope coefficient for mo	ving air [J/m3K]:					
Exponent for moving ai	[ [==];					
Pipe collector model: pip						
Pipe collector model: ou	ter diameter of pipe [mm].					
Pipe collector model: th	ermal conductivity of pipe [W/mK]:		0.4			
· Pipe collector model: he	at capacity of fluid [J/kgK]:		4180			
Pipe collector model: fra	ction of pipe included in model [%]:		100			
Model-specific outputs						
Return temperature	from pipe collector					
Total energy loss/ga	ain from entire pipe					
Inlet temperature o	f pipe collector					
		ОК	Cancel			

Figure 27: Boundary definition dialog - additional outputs of this special constraint are enabled (*PipeCollectorQdot, PipeCollectorT0, PipeCollectorTr*)

## FMU export

An FMU is created with **File-> Export Functional Mock-up Unit ....** The export dialog opens (Figure 28). In this dialog, the model name and the path to the output file can be set. In addition, the dialog contains an overview of all automatically exported input and output variables, i.e. FMU variables.

The FMU variable names must not contain spaces, so all spaces are replaced by \_. In the example shown, the output file definitions **Temperature 0.5 m** and **Temperature 1.0 m** have been renamed accordingly to **Temperature\_0.5\_m** and **Temperature\_1.0\_m**.

After confirming the dialog with "Create FMU", the FMU can be used in a co-simulation master program.

Physical units of the FMI variables: The units for the FMI interface variables are defined in the case of input variables according to their physical quantity. For automatically generated output variables (see example tube collector above), the units are also determined according to their physical quantity. For output variables, the unit is set in the output definition dialog.

		FMU-Export		6
odellname:	PipeCollector			
usgabeverzeichnis für generierte	FMU: /tmp/PipeCollector.fm	/tmp/PipeCollector.fmu		
ngangsvariablen:				
Alle Klimabedingungen mit dem '	Typ "External" werden Eingar	ngsvariablen (vom Typ real).		
Variablenname	Bedingungstyp	Einheit		
ClimateCond.Vorlauftemperatur	Temperatur [Temperature]	c		
gebnisgrößen: Alle Ausgabedefinitionen, welche	skalare Werte schreiben, we	erden Ergebnisgrößen (vom Typ real).		
gebnisgrößen: Alle Ausgabedefinitionen, welche Variablenname	skalare Werte schreiben, we	erden Ergebnisgrößen (vom Typ real). Ausgabegröße	Einheit	
gebnisgrößen: Alle Ausgabedefinitionen, welche Variablenname Temperatur_0.5_m	skalare Werte schreiben, we Temperatur [Temperature]	erden Ergebnisgrößen (vom Typ real). Ausgabegröße	Einheit	
rgebnisgrößen: Alle Ausgabedefinitionen, welche Variablenname Temperatur_0.5_m Temperatur_1.0_m	skalare Werte schreiben, we Temperatur [Temperature] Temperatur [Temperature]	erden Ergebnisgrößen (vom Typ real). Ausgabegröße ] ]	Einheit C C	
rgebnisgrößen: Alle Ausgabedefinitionen, welche Variablenname Temperatur_0.5_m Temperatur_1.0_m Rohrkollektor-PipeCollectorT0	skalare Werte schreiben, we Temperatur [Temperature] Temperatur [Temperature] Einlasstemperatur des Roh	erden Ergebnisgrößen (vom Typ real). Ausgabegröße ] ] hres [PipeCollectorT0]	Einheit C C C	
rgebnisgrößen: Alle Ausgabedefinitionen, welche Variablenname Temperatur_0.5_m Temperatur_1.0_m Rohrkollektor-PipeCollectorT0 Rohrkollektor-PipeCollectorTr	skalare Werte schreiben, we Temperatur [Temperature] Temperatur (Temperature] Einlasstemperatur des Roh Ausflusstemperatur des Roh	erden Ergebnisgrößen (vom Typ real). Ausgabegröße ] ] hres [PipeCollectorT0] ohres [PipeCollectorTr]	Einheit C C C C	
rgebnisgrößen: Alle Ausgabedefinitionen, welche Variablenname Temperatur_0.5_m Temperatur_1.0_m Rohrkollektor-PipeCollectorT0	skalare Werte schreiben, we Temperatur [Temperature] Temperatur [Temperature]	erden Ergebnisgrößen (vom Typ real). Ausgabegröße ] ] ] nres [PipeCollectorT0]	Einheit C C	
rgebnisgrößen: Alle Ausgabedefinitionen, welche Variablenname Temperatur_0.5_m Temperatur_1.0_m Rohrkollektor-PipeCollectorT0 Rohrkollektor-PipeCollectorTr Rohrkollektor-PipeCollectorQdo	skalare Werte schreiben, we Temperatur [Temperature] Temperatur [Temperature] Einlasstemperatur des Roh Ausflusstemperatur des Ro t Gesamtenergieverlust/-gen	erden Ergebnisgrößen (vom Typ real). Ausgabegröße ] ] hres [PipeCollectorT0] ohres [PipeCollectorT7] winn des gesamten Rohres [PipeCollectorQdot]	Einheit C C C C W	

#### Figure 28: FMU-export dialog - in the lists the input variables and output quantities are shown.

The yellow-backed outputs in Figure 28 are the variables generated from special models. The name of this is composed of the name of the boundary condition / field condition (here tube collector) and the physical quantity. The units of automatically generated quantities are fixed. The units of the self-defined outputs (here *temperature\_0.5\_m* and *temperature\_1.0\_m*) correspond to the units selected in the output definition dialog.

# 3.3.4 Co-Simulation examples

A first example of co-simulation "Divided wall" is available in the DELPHIN 6 tutorial "FMI Co-Simulation with DELPHIN 6"<sup>41</sup>. It describes following steps in detail:

<sup>&</sup>lt;sup>41</sup> Tutorial available from <u>https://cloudstore.zih.tu-dresden.de/index.php/s/PiPxDn6kt2AkGFJ</u>

- Export of the complete wall as FMU
- Import of the DELPHIN FMU with the complete wall model into the co-simulation master program MASTERSIM
- Import of the left-side wall model and test calculation with specified external temperatures
- Import of the right-side wall model and use of a signal inverter FMU

# 3.4 Remaining gap between research and practice

The transfer of knowledge or the practical integration of research results is a process that requires cooperation between universities, institutes, companies, intermediaries and even governments. Good teamwork is the key to successful industrialization and commercialization of scientific and technological achievements. This section reviews the current mechanisms for collaboration in knowledge transfer. Where appropriate, appropriate methods need to be developed to improve the practical integration of tools developed in the field of science.

In planning practice, energetic optimization potentials can often not be sufficiently exploited, because broadbased planning tools are not designed for this purpose. The lack of reliable data also represents a major obstacle to the prioritization, planning and implementation of energy supply concepts for settlements and neighborhoods. It is only possible in exceptional cases and with high time and expense to investigate the dynamic behavior of buildings and facilities using simulation programs. Variant analyzes under energetic operational optimization criteria have not yet been established as standard for cost reasons.

Planning tools	Research tools			
Practice oriented development, Customized implementation of localized standards, Extensive standard data sets	Project motivated tool development and data collection, Flexible development technologies, Diverse programming languages, Model diversity			
Professional graphical user interface(GUI) and post process tool, Software speed and convenience sensitivity, Sufficient documentation	Rare professional graphical user interface (GUI) and post process tool, Less concern of calculation speed, Inadequate documentation			
Profit-oriented marketing, Powerful service and education after sale	d Mostly in-house use, No commercial exploitation Little support for outsiders			
No tool integration, Increasingly valued BIM	Little tool integration and BIM			

#### Table 8: Research and planning tools comparison

There is also a lack of practicable methods for comprehensively determining the input data. Input and model parameters are not yet known in the early planning stages or have unknown or major uncertainties. Practical standard values for user profiles, design variants or systems engineering as well as methods for their uncertainty evaluation and sensitivity analysis are not sufficiently available or, due to their complexity, only available as expert or research systems. Similarly, the criteria developed so far for evaluating the quality of the simulation results should be extended in order to improve the predictive accuracy between calculated and real energetic building behavior.

Since no general quality standards of software developments have been defined among the various research and demonstration projects, there are hardly any interfaces between the tools, and coupling is largely

impossible. In conclusion, it can be stated that improved overall coordination in the development of planning instruments from publicly funded projects is necessary in order to respond adequately to current challenges and avoid costly duplication.

While there is active collaboration between research institutions and companies in the development of building simulation tools, only specialized and technological issues are concentrated. Collaboration at the macroscopic level is rare. The demand for interdisciplinary modeling, cross-criteria analysis and lifecycle integration goes far beyond current individual collaboration. Table 8 shows some obvious differences between planning and research tools. This comparison clarifies how the gap between research and practice could be bridged.

# 3.5 Proposal of a knowledge transfer platform

As shown in Figure 29, new transfer mechanisms between research and practice need to be established to better organize the flow of information. This should help to facilitate the communication between all participating domains and organizations in a flexible and efficient way.



Figure 29: Knowledge integration and transfer demands from research to practice

The overall objective of the Transfer Platform, shown in Figure 30 (Grunewald et al., 2015), is to translate the scientific methods and procedures into reliable tools that can be used in practice and thus to integrate them economically into the planning process. The preparation of scientific results for practical application usually requires a focus on the crucial issues (e.g., reduction of complexity). This is done by evaluating and transforming free research tools from the scientific level and integrating them into the networked simulation environment of the Transfer Platform. Appropriate standards and protocols should be developed to ensure the interoperability of newly integrated research tools.

The Transfer Platform establishes an additional layer between research and practice across the lifecycle of buildings, settlements and cities. The main features of the Transfer Platform are:

- Publicly available free platform
- Maximum bundling of development capacities
- Interoperability (co-simulation and model exchange)
- Development of uniform standards (programming, interfaces, licensing)
- Data and model-side integration of the building information models
- Cross-domain energy efficiency technologies for components, plants, buildings and settlements
- Processing through model reduction and calculation time optimization
- Data consistency and completeness: plausibility, calibration & validation
- Internationalization through purely physical modeling principles

## Non-profit marketing to secure support



Figure 30: Definition of a Transfer platform in the area of interdisciplinary performance analysis of buildings, neighborhoods and cities

At the same time, Transfer-Platform serves the development and provision of scientifically proven reference solutions under the following premises:

- The sub-models are maintained by the subject-specific competence partners in order to be able to keep abreast of current developments in practice and science in view of the variety of models.
- Building information models ensure consistent and lossless data flow throughout the lifecycle. Planning data can be used to optimize the operation.
- It is possible to work according to the processing progress at the appropriate modeling depth.
- Simulation models of different applications (building model, plant-technical model, and control model) can be combined via interfaces.
- Models are scalable depending on the level of detail (component, building, settlement, and grid).
- Models of different domains (e.g., hydraulic, thermal, electrical) can be combined.
- Statistical methods for uncertainty assessment allow statements about the variance of the simulation results.

For the Transfer Platform, it is important to shift the focus away from traditional single tool development to network-coordinated collaboration. Maximum synergy effects are sought, which is promoted by a close networking of science and practice.

The implementation of the upcoming tasks in high-quality physical-mathematical models is a priority task of the scientific development teams. User-friendly program interfaces, on the other hand, can only be developed to a limited extent by the research partners. The resources must be used specifically for research tasks. Sales, support and marketing, for example, should be provided by commercial software companies. A clear division of labor between science and practice is seen as a prerequisite for achieving the goals formulated above.

The technological implementation of the Transfer Platform has to be bundled on a central server, which offers several advantages:

- Interfaces are better coordinated between the scientific institutions.
- Specialist planners get easily access to scientifically maintained tools.
- The planning tools on the model platform are kept always up to date.
- The development of a distribution system by the research institutions is not necessary.
- Projects for further development can be tailored precisely.
- The visibility of research funding is increased.

In addition to the model platform, a data repository for validated input data is needed. In an integral planning process, the level of detail of a model depends on the stage in the planning. In the early design or planning phase, many parameters are still unknown. In order to be able to make decisions in this phase, meaningful default values for user profiles, design data, system data and location data must be available that match the respective detail level of the model.

# 3.6 The need to change the financing policy

The current funding policy for energy efficiency of buildings and neighborhoods focuses mainly on application-based projects, where tool development is mostly just a sub-item. This does not correspond to the importance that it should have in construction. Such a funding policy is not expedient from the point of view of the development of simulation tools. A well-designed funding policy should motivate developers to network to serve longer-term goals rather than looking too quickly for commercial exploitation.

On the other hand, the funding policy should motivate software manufacturers to prefer to integrate highquality scientific solutions into their products instead of only implementing what has already been formulated in standards. This would accelerate the transfer of knowledge. It is important to note that collaboration between research and practice is a long-term process and that continuous funding to ensure continuity must be ensured.

The new thinking of research funding in the field of energy-efficient buildings and neighborhoods must be supported by appropriate legislation. There is a good opportunity for this in Germany, where the new building energy law is being publicly discussed with the participation of many associations. Currently, the Energy Saving Act (EnEG), the Energy Saving Ordinance (EnEV) and the Renewable Energy Heat Act (EEWärmeG) should be combined to a new Building Energy Act (GEG).

Fundamental criticism addresses the missing perspective for climate-neutral and sustainable building stock 2050. The present draft of the GEG does not provide sufficient incentives to achieve the climate protection goals. To get close to these goals, an ambitious roadmap / destination path needs to be developed.

It is counterproductive to regulate a large number of minimal individual aspects with great depth of detail. More flexible and open-to-technology goals should be addressed, less detailed targets. The decision on the method of implementation should be left to the building owners or the parties involved in the planning process.

The present draft of the GEG lacks a vision on the evolution of calculation methods. Not only do they have to keep pace with technological progress, but they should also, as is common in other disciplines, play a leading

role in the development of energy supply concepts. The present draft of the GEG does not sufficiently respond to the challenges of digitization, e.g. there are no statements about Building Information Modeling (BIM). It is expressly pointed out that the entire lifecycle of the buildings must be considered. In the long term, instruments need to be developed to assess the energy and resource use of buildings and facilities not only for operation, but also for production and disposal (consideration of "embodied energy").

The goal is to reduce the real energy consumption, not the one predicted during the planning. To be able to learn from mistakes requires a systematic comparison of demand and consumption certificates. Since a performance gap exists in many cases, a consumption certificate should be compulsory after the completion of a building. This can be done in the first 5 years (possibly again at user / utilization change). This consumption certificate should then be the basis for promotion and demand measures for the building owners as well as the legislator.

At the same time, the client can use the difference between actual energy consumption and planned consumption in order to check the quality of the energy planning as well as the structural implementation in order to be able to assert a recourse claim in the event of extreme deviations. This leads to the desired increased planning and execution quality and planners will endeavor to use appropriate planning tools and calculation methods. Thus, an evolution of the calculation methods and planning software is already motivated by market mechanisms.

# 4 Common exercises on the basis of PASSYS cells

In the previous chapters of this report, a gap analysis was performed from a general perspective. Since single features of the simulation programs were not discussed in detail, this general approach is to be supplemented by a more detailed analysis of individual simulation tools. Common exercises were defined and solved and the comparison of the results revealed strengths and weaknesses of the programs used.

The common exercises have been defined for two different groups of simulation tools, both of them cover important aspects in the context of the whole building performance simulation:

- 1) programs for simulation of the hygrothermal performance of building envelope constructions (2D),
- 2) programs for simulation of the multi-zone energy performance in whole buildings (3D).

The basic difference between these two program groups is that building envelope simulation programs normally simplify the 3D problem in 2D, but consider more complex physical relationships, e.g. they take into account transient coupled energy and mass flows and use completely discretized constructions. In contrast, multi-zone building energy programs generally use simplified 3D building models in which the walls are idealized as simple 1D problems and the coupling of the processes cannot be taken into account to the same extent.

The modeling approaches of these two program groups are very different. Building envelope simulation programs examine details of construction with a focus on durability and moisture-related damage, while multi-zone building energy programs evaluate the overall building performance with a focus on energy efficiency. This must be taken into account when comparing the results between these two groups.

Therefore, prior to the start of the official common exercises, a pre-evaluation was carried out to compare the results of these two groups. Specially adapted PASSYS variants were created and simulated with DELPHIN6 and NANDRAD. For example, the back and front walls have been left out in NANDRAD to simulate 2D cases. In addition, spatially averaged output quantities were used in DELPHIN6 to output the same physical quantities as in NANDAD. In summary, it was found that the differences between DELPHIN6 and NANDRAD were very small if the projects were defined in such a way that the results are correctly comparable.

# 4.1 Model of the PASSYS cell

The common exercises were built upon the PASSYS Cells Project (Wouters, Vandaele et al., 1990). PASSYS test cells are identical test facilities implemented in different locations in Europe to test the performance of different wall constructions and their influence on indoor climate under real climatic conditions. A photo and a sketch of a PASSYS cell are shown in Figure 31, which consists of a test room and a service room, separated by a partition wall. A sectional view is shown in Figure 32. The test room is equipped with an exchangeable external wall at its front side.

The purpose of the common exercises was comparison of different simulation programs. Therefore, the original construction of the PASSYS cell could be adapted to fit the requirements of the exercise. Construction boards consisting of rigid PS-foam insulation material and steel covering were used, see Figure 33. The cell was put up using 100 mm thick insulation panels reinforced by H-steel beams. Additional 300 mm thick insulation boards were used as a partition to separate the test room. Concrete foundation and support construction were neglected (see Figure 33).



Figure 31: PASSYS cells photo and sketch



Figure 32: Sectional view of the PASSYS cell (Wouters, Vandaele et al., 1990).



Figure 33: 2D simulation model of the PASSYS cell. The orientation of cells in this model is east (right) to west (left).

# 4.2 Boundary conditions and climate data

The climate data of the city of Essen, Germany - hourly values of temperature, relative humidity, direct and diffuse solar radiation, atmospheric counter radiation, wind velocity and direction, and rain provided by the German weather service (DWD) were used for all variants. For calculation of the radiation flux and the rain load intensity, the geographical data of the location Essen is given in Table 9.

#### Table 9: Geographical data of Essen

Name	Value	
Latitude	51.456	
Longitude	7.012	
Elevation above mean sea level	26.5 – 202.5 m	

#### Test Reference Years (TRY) in Germany

Temperature Relative humidity

Wind velocity Wind direction

Rain (from old TRY)

Direct sun radiation Diffuse sun radiation

Atmospheric counter rad

Source: Deutscher Wetterdienst

Cyclic annual data on hourly basis:

- 1 Bremerhaven
- 2 Rostock
- 3 Hamburg
- 4 Potsdam

# 5 - Essen

- 6 Bad Marienber
  - Bad Marienberg
- 7 Kassel
- 8 Braunlage
- 9 Chemnitz
- 10 Hof
- 11 Fichtelberg
- 12 Mannheim
- 13 Passau
- 14 Stötten
- 15 Garmisch-Partenkirchen



#### Figure 34: Location and climate data

A constant ground temperature of 8 °C was used as a boundary condition at the bottom side. The initial conditions of 20 °C and 80 % RH were the same for all test cases. The total simulation time was 365 days. The boundary conditions were assigned to the construction as indicated in Figure 35.

The climate data and additional parameters as solar absorption, heat emission, convective heat transfer and moisture absorption coefficients are used to calculate the heat and moisture flows at the boundaries of the construction. The orientation of the construction elements had to be taken into account for radiation and rain flux.



DIRRAD

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Figure 36: Climate data of TRY Essen given on hourly basis for a full year

# 4.3 2D exercise of building envelope simulation programs

Since there are not many hygrothermal building envelope simulation tools available worldwide, the selection was limited to the tools developed and maintained by the participants of the Annex 68: CHAMPS-BES<sup>42</sup>, DELPHIN5 and DELPHIN6<sup>43</sup>, see Figure 37.

## CHAMPS-BES1.7.1 (2007)

Coupled HAM-simulation tool for building envelope systems including VOC adsorption and emission, Limitations: free air spaces, old materials DB, rudimentary VOC DB, 2D

## DELPHIN5.9.2 (2017)

Coupled HAM-simulation tool for building envelope systems including VOC adsorption and emission, new materials DB, extended VOC DB, improved air flow model, Limitations: 2D

DELPHIN6.0.13 (2017)

Coupled HAM-simulation tool for building envelope systems, 3D modeling possible, essentially improved numerical engine, parallelized solver, completely re-designed GUI, Limitations: no VOC implemented yet







#### Figure 37: Building envelope simulation programs used for the 2D common exercise

CHAMPS-BES has been developed at the Syracuse University in 2006-2007 on the basis of the former DELPHIN4 versions (1987-2006). In fact, CHAMPS-BES is identical to a very early DELPHIN5 version. The DELPHIN5 development continued at the TU Dresden until 2017. During this time, many updates and new features were implemented. DELPHIN6 is a major upgrade of DELPHIN5, the first version has been released in 2017. It comes with a completely re-designed parallelized simulation engine, which runs much faster especially in case of large problems, and it has a newly designed multi-lingual and multi-platform graphical user interface. In addition to DELPHIN6, a specially tailored scientific post processing tool POSTPROC has been developed which greatly facilitates the analysis of simulation results.

All programs, CHAMPS-BES, DELPHIN5 and DELPHIN6, allow to select the desired output from a list of predefined physical quantities. For the purpose of the common exercise, following outputs were identically selected in each program:

- 1. test / service room
  - average room air temperature and relative humidity
- 2. each wall / roof / floor construction

<sup>&</sup>lt;sup>42</sup> http://champs.syr.edu/software/champs\_bes.html

<sup>&</sup>lt;sup>43</sup> http://www.bauklimatik-dresden.de/index.php?aLa=en

- average temperature and relative humidity at three locations (inside, middle, outside)
- 3. whole construction
  - integral moisture content (sum of all moisture in rooms and constructions)
  - fields of temperature, relative humidity and water content (in each single cell according to discretization)

Single output values are usually reported on hourly basis. Fields are reported on larger output intervals (e.g. 2.5 d) in order to avoid extremely big output files.



Figure 38: Selected outputs of building envelope simulation programs; the red lines indicate spatially averaged quantities over the lengths of the construction elements in different depths.

The modelling complexity is gradually increased in five steps. It starts with pure thermal analysis (H) and hygrothermal analysis (HM) followed by hygrothermal analysis with airflows (HAM). Finally, emission analysis is added to the previous test cases (HAMP). Each of the test cases includes sub-cases as shown in the list below, which will be executed according to the individual modelling capabilities of the tested tools. During the course of the Annex 68 project, the test cases printed in bold letters could solved and evaluated. The results are documented and compared in Appendix 1 of this report.

Initial plan to increase the complexity of the exercise:

- 1) Thermal analysis (H)
  - a. Free-running building, just heat transfer through walls
  - b. External long-wave and short-wave radiation
  - c. Internal heat sources, internal long-wave radiation
- 2) Hygrothermal analysis (HM)
  - a. Moisture fluctuation in rooms
  - b. Rain load, capillary action and moisture buffering in walls
  - c. Internal moisture sources
- 3) Hygrothermal analysis with air flows (HAM)
  - a. Air exchange with external air in zones
  - b. Air permeable construction elements, air flow between zones
  - c. Air flow within zones, buoyancy effects
- 4) Emission analysis (HAMP)
  - a. Internal VOC sources in zones
  - b. Absorption and emission of VOC by construction materials
  - c. Combination of internal VOC sources, absorption and emission
  - d. Scheduled ventilation

- e. Demand-controlled ventilation
- f. Influence of heating and cooling, energy optimized HVAC operation

# 4.4 Summary of the 2D common exercise

The different strengths and weaknesses of the tested programs revealed in the 2D common exercise must be seen in the light of their level of development. The good news is that all three programs have a solid numerical basis that enables the simulation of coupled transient hygrothermal problems in building envelope systems. Apart from the fact that the driving rain model has been updated in DELPHIN6, which leads to slight deviations, all programs deliver identical results.

The consideration of air spaces changes this picture. CHAMPS-BES was developed in 2 years and has not been further developed since 2007. Instead, many bug fixes and improvements have been implemented in DELPHIN5, including correct implementation of the moisture mass balance in airspaces. This explains why CHAMPS-BES deviates when calculating the relative humidity in the service and test rooms. The error in the moisture mass balance not only led to incorrect results, but also slowed down the simulation speed. Therefore CHAMPS-BES had to be removed from the further analysis with air flows.

The variants including air flows could be solved by DELPHIN5 and DELPHIN6. However, such fully coupled problems are much more demanding in terms of simulation time. These cases showed a clear advantage of DELPHIN6 over DELPHIN5. In order to make a comparison, the size of the PASSYS cell had to be reduced. With a small and a very small version of the PASSYS cell, all simulation variants could be accomplished by DELPHIN5 and DELPHIN6.

The comparison of results between DELPHIN5 and DELPHIN6 delivered good results for most but not all cases. Unresolved deviations in moisture contents were observed in case of air change dominated drying periods, which should be taken into consideration for future updates of the DELPHIN software.

An emission analysis was not possible as part of the exercise, as features in VOC transport and emission analysis and database management were missing in both programs, DELPHIN5 and DELPHIN6. These functions had to be implemented before the exercise could continue. Since the development of DELPHIN5 ended in 2017, it made sense to concentrate on DELPHIN6 with new implementations. The VOC functions newly implemented in DELPHIN6 are documented in sections 5.1 - 5.3.

With the new version of DELPHIN6 as the only remaining tool, the common exercise could be completed, see section 5.7. Isothermal and non-isothermal emissions from a material's source of pollutants were simulated in the test room of the PASSYS cell. An initially high concentration of Hexanal was assumed in the floor plate of the test room, while an air exchange rate of 0.2 per hour was compared to no ventilation. All results from the new DELPHIN6 version look reasonable and meet the expectations.

# 4.5 3D whole building simulation exercise

A second common exercise was carried out to enable a comparison between several programs for simulation of the multi-zone energy performance in whole buildings (3D), in which the strengths and weaknesses of each individual program were determined. For this purpose, 8 different categories with different test cases were developed to examine individual physical effects in detail. On this basis, possible problems and restrictions can be made effectively visible and a validation report can be created.

In order to achieve a wide range of results, 6 different participants, who modeled the test cases with different building simulation tools, took part in the common exercise, so that a wider range of different tools could be evaluated.

Program	Version	Editor
NANDRAD	NANDRAD 1.7 (Inhouse Version)	Stephan Hirth, TU Dresden
Energy Plus	Energy Plus 8.6	Stephan Hirth, TU Dresden
Modelica	Dymola 2019, Modelica 3.2.2, 2.0.0	Klaas De Jonge, Universiteit Gent
IDA ICE	4.8 SP1	Jakub Kolarik, DTU Copenhagen
DYNBIL	0.19.8.	Gabriel Rojas-Kopeinig, Universität Innsbruck
TRNSYS	18	Jelle Laverge, Universiteit Gent

Table 10: Thermal Building Simulation Tools that took part in the Common Exercise

The 3D model of the PASSYS cell consists of two rooms, a test room (5 m x 2.76 m x 2.75 m) and a service room (2.40 m x 3.32 m x 3.33 m), see Figure 39. All dimensions in the geometry model relate to internal dimensions.



Figure 39: Geometric 3D model of the PASSYS cell

# 4.6 Overview of test cases

The aim of this exercise is to include the widest possible range of validation cases in the investigation. In order to systematize the variety of test cases, the following eight test categories were defined:

- 1. Construction
- 2. Outdoor Climate
- 3. Indoor Climate
- 4. Internal Loads

- 5. Infiltration
- 6. Heating/Cooling
- 7. Hygrothermal
- 8. Pollutants

Table 11 provides an overview of all test cases with a brief description of the individual test cases. It also lists all programs that took part in the common exercise. Each test case that has been completed by a specific program is marked with an  $\times$  in the table.

Category	ID	Test Case	NANDRAD	Energy Plus	IDA ICE	TRNSYS	Modelica	DYNBIL
Initial	T100	Base Case	×	×	×	×	×	×
Construction	T201	Heavy Construction	×	×	×	×	×	×
	T202	Ground Contact	×	×	×	×	×	×
	T203	Window	×	×	×	×	×	×
	T204	deleted				-		
	T301	Short-wave radiation	×	×	×	×	×	×
Outdoor	T302	Long-wave radiation	×	×	×	×	×	×
Climate	T303	Convection coefficient		×	×	×	×	
	Т304	Combination of T301, T302 and T303		×	×	×	×	
	T401	Long-wave radiation	×	×	×	×	×	×
	T402	deleted				-		
	T403a	Simple window model without angle dependence	×		×	×	×	×
Indoor	T403b	Simple window model with angle dependence	×			×		
Climate	T404	Combination of T401 and T403b (if not available T403a)	×			×	×	×
	T405a	Detailed window model with angle dependence	×	×	×	×	×	×
	T405b	Detailed Window Model with angle dependence and internal radiation distribution	×			×		×
Internal Loads	T501	Internal Heat Loads	×	×	×	×	×	×
	T502	Internal Heat Loads with convective/radiative split	×	×	×	×	×	×
	T601	Constant Infiltration	×	×	×	×	×	×
	T602a	Infiltration defined by design flow rate – temperature driven		×	×	×	×	×
	T602b	Infiltration defined by design flow rate – wind driven		×	×	×	×	×
Infiltration	T602	Infiltration defined by design flow rate – wind & temperature driven		×	×	×	×	×
	Т603	Wind speed and stack effect dependent infiltration			×	×	×	×
	T604	Overflow case			×	×	×	×

Table 11: Overview of all test cases and which program took part in which test case (marked with an X)
	T605	Realistic Test Case: Combination of T602 and T604			×	×	×	×
Heating/ Cooling	T701a	Constant ideal heating	×	×	×	×	×	×
	T701b	Constant ideal cooling	×	×	×	×	×	×
	T701	Ideal Heating/Cooling	×	×	×	×	×	×
	T702	Surface Heating/Cooling					×	×
Hygro- thermal	T801	Include moisture balance without moisture source			×	×	×	×
	T802	Include moisture balance with moisture source (schedule)			×	×	×	×
	T803	Include moisture balance with moisture source and buffer effects				×		×
	T901	Include inert pollutant (CO2)				×	×	
Pollutants	T902	Combine inert pollutant (CO2) with natural ventilation				×	×	
	Т903	Include pollutant (Hexanal) – constant climate outside						
	T904	Include pollutant (Hexanal) – variable climate outside						

Test case T903 "Include pollutant with temperature and humidity dependent source strength (Hexanal) – constant climate outside" and Test case T904 "Include pollutant with temperature and humidity dependent source strength (Hexanal) – variable climate outside" are only solved by DELPHIN6 and therefore not in part of the 3D exercise.

Unless otherwise stated in individual cases, the climate data for each test case are specified by the Essen site, which has already been described above. Predefined output values are evaluated on an hourly basis for each test case.

# 4.7 Evaluation methods

The following steps were defined to evaluate the simulation results. It should also be determined how well the results of the building simulation programs match.

- 1. Short description of each test case
- 2. Graphical analysis e.g. of the Test Room Air Temperature curve (or heating energy curve etc.) to get an visual overview of the data of each program
- 3. Numerical Analysis of the absolute Tolerance, Root Mean Square Error, Coefficient of variation of the RMSE, Mean Bias Error and the total error between two programs (see below).
- 4. For each test case there is a notes section for certain matters that were noticed during the evaluation process.

In order to be able to visually compare the results of the participating programs and thus qualitatively analyze their different behavior, different graphs are automatically generated for each test case (see Figure 40).



Figure 40: Example for a graph for the Air Temperature of the test room for the base case T100

All formulas for numerical analysis are listed below:

Absolute tolerance:  $Tol, abs = \max(T_{air,prog,t} - T_{air,prog,ref,t}); t \ge 240h (10 \text{ days for transient oscillation})$ 

Residual:  $Residual_t = T_{air,prog,t} - T_{air,prog,ref,t}$ 

Root Mean Square Error (RMSE) and Coefficient of variation of the RMSE, CV (RMSE):

$$RMSE = \sqrt{\frac{\sum_{t=1}^{n} (Residual_{t})^{2}}{n}} \qquad CV(RMSE) = \frac{RMSE}{T_{aur}}$$

Mean Bias Error (MBE) and Total error:

$$MBE = \frac{\sum_{t=1}^{n} (Residual_t)}{n} \qquad Error_{Total} = \sqrt{RMSE^2 + MBE^2}$$

For a short overview of the results and their quality of convergence the coefficient of variation of the root mean square error (deviation) was used since its result is unit-independent and thus it is a strong and qualitative comparison criterion.

CV (RMSD)	Quality of Similarity	
< 5 %	++	
5 – 10 %	+	
10 – 20 %	-	
> 20 %		
Did not participate in test case	0	

Table 12: Scale for the analysis based on the coefficient of variation of the RMSE

Since different programs are compared here and the exact solution is unknown, a reference must be defined for the percentage deviations in the results. This does not mean that the reference solution is better than the others. In most test cases, NANDRAD serves as a reference. If NANDRAD does not take part in a specific test case, the reference program is marked with ref in the table. For each test case there is a diagram in which all numerical analysis criteria are shown with the same unit on the left axis as in the graphic on the left axis.



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Analysis - T100 Base Case

## 4.8 Summary of the 3D common exercise

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A categorization of existing models has been carried out based on the results of the common exercise. The test scenario was created by reusing the test cells from the PASSYS cell project. Based on a base case scenario, detailed test cases with eight different categories addressing Construction, Outdoor Climate, Indoor Climate, Internal Loads, Infiltration, Heating/Cooling, Hygrothermal construction properties and Pollutant emissions were defined. To cover a wide range of tools, six programs NANDRAD, EnergyPlus, IDA ICE, TRNSYS, Modelica and DYNBIL were used to simulate the test cases by different participants of the Annex 68.

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Good correlations between the programs have been reached for the simple base case scenarios in the construction category, e.g. free-running test cells with just heat conduction trough the walls. For more complex test cases it is necessary to keep the information in the document with the described test cases as accurate as possible and thus prevent incorrect modelling by different participants. Unfortunately, some inaccuracies have been found in the description of more complex test cases. These are mainly in the category ventilation, hygrothermal and pollution. Unfortunately, to eliminate these inaccuracies and to have all test cases redone by all participants needs several iterations and hence more time. It could therefore not be carried out within the project. It is noted in each test case if the specific test case has some inaccuracies. However, these empirical values can be used to avoid errors in future validation tasks such as the SIMQUALITY project.

In order to be able to evaluate individual strengths and weaknesses of the considered building simulation programs, an overview of all test cases can be found in Table 14. This table shows all considered programs with their deviation from the reference program in each test case. Furthermore it is indicated whether the description of the respective test case was inaccurate (highlighted with \*) and which program served as the reference (marked with *ref*).

The overview shows that differences between the programs increase the more complex the individual test cases and its tested physical effects become. For complex test cases, it is necessary to question which program (or programs) represent the correct solution and how it is to be determined for cross program checks.

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However if there are large deviations between programs, it is not possible to determine in detail where the deviations to the reference program come from. These differences can be caused by different models, different model implementations or errors in the model or implementation itself. More detailed investigations are necessary to narrow down the cause. This approach only shows that there are certain deviations and that that there is a need for a deeper examination. This should be done by someone who can deeper investigate the program and if necessary, also its source code.

Category	ID	ID Test Case		Energy Plus	IDA ICE	TRNSYS	Modelica	DYNBIL
Initial	T100	Base Case	ref	++	++	++	++	++
	T201	Heavy Construction	ref	++	++	++	++	++
Construc-	T202	Ground Contact	ref	+		++	++	++
tion	T203	Window	ref	++	+	++	++	++
	T204	deleted						
	T301	Short-wave radiation	ref	++	+	+	++	++
Outdoor	T302	Long-wave radiation	ref	++	-		+	++
Climate	Т303	Convection coefficient	ref	++	+	++	++	0
	T304	Combination of T301, T302 and T303	0	ref		+	+	+
	T401	Long wave radiation	ref	++	+	++	++	++
	T402	deleted						
	T403a	Simple window model without angle dependence	ref	0	-			+
Indoor	T403b	Simple window model with angle dependence	ref	0	0	++	+	0
Climate	T404	Combination of T401 and T403b (if not available T403a)	ref	0	0	+	+	
	T405a	Detailed window model with angle dependence	-	+	ref		+	
	T405b	Detailed Window Model with angle dependence and internal radiation distribution	ref	0	0		0	++
Internal Loads	T501	Internal Heat Loads	ref	++	+	++	++	++
	T502	Internal Heat Loads with convective/radiative split	ref	++	+	++	++	++
	T601	Constant Infiltration	ref	++	+	++	++	++
	T602a	Infiltration defined by design flow rate – temperature driven	0	++	+	ref	+	++
	T602b	Infiltration defined by design flow rate – wind driven	0	++	++	ref	++	++
Infiltration	T602	Infiltration defined by design flow rate – wind & temperature driven	0	++	++	ref	+	++
	T603	Wind speed and stack effect dependent infiltration	0	0	+	ref	++	++
	T604	Overflow case*	0	0		ref		
	T605	Realistic Test Case: Combination of T602 and T604*	0	0	+	ref	++	-
	T701a	Constant ideal heating	ref	++/++	++/-	++/++	+/-	++/-
Heating/	T701b	Constant ideal cooling	ref	+/-	+/	++/++	/++	++/++
COOMING	T701	Ideal Heating/Cooling	ref	++/++/++	++/-/-	++/++/++	-/-/+	++/++/++

#### **Table 14: Overview of test case results**

	T702	Surface Heating/Cooling	0	0	0	ref	//	0
	T801	Include moisture balance without moisture source*	0	0		ref	++	++
Hygro- thermal	T802	Include moisture balance with moisture source* (schedule)	0	0	-	ref		+
	T803	Include moisture balance with moisture source and buffer effects*	0	0	0	ref	0	-
Pollutants	Т901	Include inert pollutant (CO2)*	0	0	0	ref		0
	T902	Combine inert pollutant (CO2) with natural ventilation*	0	0	0	ref		0
	Т903	Include pollutant (Hexanal) – constant climate outside	0	0	0	0	0	0
	T904	Include pollutant (Hexanal) – variable climate outside	0	0	0	0	0	0

In order to provide a final overview, Table 15 gives a rough outline of the strengths and weaknesses of each program. It outlines the test categories and some specific test cases in which the programs achieved consistent or more divergent results from the reference program. However, it is always possible that deviations are also caused by incorrect user input and thus different model parameterizations.

Program	Strengths (Category)	Weaknesses (Category)	Note
NANDRAD	Constructions Outdoor Climate Internal Loads Construction	Infiltration Hygrothermal Cat. Pollutants	No complex Infiltration No Hygrothermal No Pollutants
Energy Plus	Construction Outdoor Climate Internal Loads Infiltration Heating/Cooling		No Hygrothermal No Pollutants
TRNSYS	Construction Heating/Cooling Internal Loads Hygrothermal	Long-Wave Radiation Convection Coefficient	No detailed Window Model test cases
IDEAS Modelica	Construction Internal Loads Infiltration	Infiltration Indoor Climate Heating/Cooling	No Pollutants
IDA ICE	Construction Internal Loads Infiltration	Indoor Climate Heating/Cooling Ground Contact	No Pollutants
DYNBIL	Construction Outdoor Climate Internal Loads Heating/Cooling Hygrothermal	Indoor Climate	No Pollutants

#### Table 15: Short list of weaknesses and strengths

# **5** New implementation steps to existing tools

# 5.1 Modelling VOC/pollutant transport in DELPHIN 6

DELPHIN6 includes balance equations for pollutant transport in porous media. When simulating pollutant transport, DELPHIN6 only considers a single compound/pollutant. When investigating different VOCs in the same construction, different simulation models have to be set up, usually just by replacing the VOC/pollutant of interest. As with other balance equations, the VOC balance is enabled on demand, with the following balance equation combinations implemented so far.

$\mathbf{Symbol}$	alt. Symbol	Unit	Description
ρ		$kg/m^3$	A mass density
j		$kg/m^2s$	A mass flux density
σ		$kg/m^3s$	A mass production rate
T		K	Temperature
t		8	Time
x		m	Coordinate
$\varrho^{voc,g}$		$kg_{(VOC)}/m_{(REV)}^3$	Gas phase VOC mass density
$\varrho^{voc,s}$	$c_m$	$kg_{(VOC)}/m^3_{(REV)}$	Adsorbed VOC mass density (often also used as total VOC mass density, since it is generally much larger than the gas phase VOC mass density)
$\varrho_g^{voc}$	С	$kg_{(VOC)}/m^3_{(gas)}$	Gas phase VOC concentration, or density of VOC with respect to gas volume in porous medium
$\varrho_{g,sat}^{voc}$		$kg_{(VOC)}/m^3_{(gas)}$	Saturation gas phase VOC concentration, or saturation density
$\sigma^{voc}_{g \rightarrow s}$		$kg/m^3s$	$Phase\ transition\ rate/condensation/adsorbation\ rate\ (from\ gas\ phase\ to\ solid\ phase)$
$\sigma_{vent}^{voc}$		$kg/m^3s$	Mass production/removal rate due to ventilation
$j_{diff}^{voc}$		$kg/m^2s$	Diffusive VOC mass flux density
$j_{conv}^{voc}$		$kg/m^2s$	Convective VOC mass flux density
R		J/molK	Ideal gas constant = $8.3144598 \text{ J/molK}$
$R_{voc}$		J/kgK	Specific gas constant of the VOC/pollutant
$M_{voc}$		kg/mol	Molar mass of VOC/pollutant
$p_{voc}$		Pa	Partial pressure of VOC
$K_g$		S	Gas permeability of the material (with respect to gas pressure gradient), typically measured for dry air and used as dry air permeability
$K_m$		kg/kg	Partition coefficient, or ratio of adsorbed VOC mass over equilibrium gas phase VOC mass
$K_{voc}$		s	VOC permeability of the material with respect to a gradient of VOC partial pressure
$D_{voc,air}$		$m^2/s$	Diffusion coefficient of the VOC in air with respect to a gas phase VOC concentration gradient
$D_m$		$m^2/s$	Diffusion coefficient of the VOC in the material with respect to an adsorbed/- total VOC mass density gradient
$\mu_{voc}$		-	VOC diffusion resistance factor of the material (similar to the vapor diffusion resistance factor)
$\beta_{voc}$		s/m	Exchange coefficient for VOC diffusion mass flux across a surface with respect to difference in VOC partial pressures
$h_{voc}$		m/s	Mass transfer coefficient with respect to gas phase VOC concentration
$n_{vent}$		1/s	Ventilation rate
$k_m$		_	Transfer coefficient for phase transition rate, with respect to difference in gas phase VOC concentration

#### Table 16: List of symbols

## 5.1.1 Balance Equation Combinations

## Isothermal VOC balance (P)

When only the pollutant balance is used, the temperature across the calculation domain, and also of the ambient air, is always 23°C. Only two balance equations are simulated in the program, one for the gas phase VOCs and one for the adsorbed VOCs. This is also the fastest method of simulating VOC transport in porous media. For this method, only very few VOC related parameters are needed and there are no additional requirements on other material data.

## Isothermal VOC balance with air flow (AP)

In addition to enabling the pollutant balance, the quasi-steady air flow model can be enabled. Since this is still an isothermal simulation (again with constant 23°C), it is only meaningful for forced-flow conditions, i.e. when the construction or part of it is exposed to a pressure gradient and air flow through the construction leads to convective VOC transport. For this variant, still only two balance equations need to be solved, since the air flow pattern is only updated when necessary (quasi-steady approach).

The material property  $K_{e}$  (gas permeability) is needed for all materials with air flow enabled.

## Temperature-dependent VOC transport (HP)

Enabling energy and pollutant balances gives a coupled simulation, where temperature in the construction has an impact on VOC emission and diffusion speed. In this combination, three coupled balance equations are solved, two pollutant balances (gas and adsorbed phase) and the energy balance.

## Temperature-dependent VOC transport with air flow (HAP)

In this variant, the quasi-steady air flow model is enabled in addition to the energy and pollutant balances. Again, only three balance equations need to be solved. The air flow can now be buoyancy-driven, so there will be an even stronger interaction between thermal transport and temperature conditions, air flow and convective VOC transport. This variant is also the slowest method. Section 5.3.1 describes how these balance equations are selected in the DELPHIN user interface.

The VOC transport model is a mechanistic transport model where VOCs are transported via diffusion and convection. The model comprises several sub-models with individual parameter sets:

- Balance equation and calculation algorithm that related conserved quantities to intrinsic states and material/VOC properties (e.g. calculation of gas-phase VOC concentration, partial pressure of VOCs, VOC permeability, etc.)
- VOC diffusion boundary condition
- Initial condition calculation model
- Contact condition for specifying mass transfer coefficient between normal and air materials within the construction
- VOC sources/sinks resulting from air change with ambient air
- Phase transition between gas phase and adsorbed VOCs (emission/adsorption)
- During initialization of the simulation model, the mechanistic model parameters are computed from standardized VOC and VOC-material-parameters

#### 5.1.2 Conservation equations (balance equations)

Two balance equations are defined for pollutant transport, one for the gas phase VOC mass density (1) and one for the adsorbed VOCs (2). These quantities are the conserved quantities<sup>44</sup>. Both balance equations are coupled via emission (transfer of VOCs from adsorbed to gas phase) and adsorption (from gas to solid phase) processes, described by a phase transition term  $\sigma_{e\to s}^{voc}$ .

Transport only occurs in the gas phase, hence this is a classical mobile-immobile-phase model. Transport occurs via diffusion and convection, denoted with subscripts *diff* and *conv*, respectively.

$$\frac{\partial \varrho^{voc,g}}{\partial t} = -\nabla \left( j_{diff}^{voc} + j_{conv}^{voc} \right) - \sigma_{g \to s}^{voc} + \sigma_{vent}^{voc}$$
(1)

$$\frac{\partial \varrho^{voc,s}}{\partial t} = \sigma_{g \to s}^{voc}$$
(2)

The optional source term  $\sigma_{vent}^{voc}$  arises when air change with ambient air is considered in the model.

#### 5.1.3 Conserved and intrinsic quantities

The conserved quantities are related to intrinsic quantities, like the intrinsic gas phase VOC concentration  $\rho_g^{voc}$  (density of VOC with respect to gas volume in porous medium) and partial pressure of VOCs. The adsorbed VOC mass density is related to the intrinsic equilibrium gas phase concentration through a storage relation, commonly expressed as a linear function using the partition coefficient  $K_{ma}$  as factor (3).

$$\rho^{voc,s+g} = \rho^{voc,s} + \rho^{voc,g} = K_{ma} \rho^{voc}_{g,eq}(T_{ref})$$
(3)

This corresponds to  $C_m = K_{ma}C_a$  (a formulation typically found in literature)<sup>45</sup>. With the ideal gas law we can express the partial pressure of the VOC (4).

$$p_{voc} = \rho_g^{voc} R_{voc} T \tag{4}$$

with  $R_{voc} = R / M_{voc}$  (gas constant divided by molar mass of VOC).

#### 5.1.4 Phase transition between adsorbed and gaseous VOCs

The mobile-immobile phase model for VOCs in DELPHIN 6 includes a phase transition term  $\sigma_{g \to s}^{voc}$ . The phase transition is based on the equilibrium concentration above the adsorbed phase, defined by the storage

<sup>&</sup>lt;sup>44</sup> Note that  $\rho^{voc,s} + \rho^{voc,g}$  corresponds typically to symbol  $C_m$  and  $\rho^{voc,g}$  is *not* the gas phase VOC concentration  $C_a$ <sup>45</sup> The symbol  $C_a$  is used for the intrinsic equilibrium gas phase VOC concentration  $\rho^{voc}_{g.eq}(T_{ref})$  at reference temperature.

relation and hence by the partition coefficient. For a given adsorbed VOC concentration  $\rho^{voc,s+g}$  we obtain the equilibrium gas phase concentration  $\rho_{g,eq}^{voc}(T_{ref}) = \rho^{voc,s+g} / K_{ma}$ .

In a coupled simulation with the energy balance, the equilibrium gas phase concentration becomes a temperature dependent quantity. Typically, for higher temperatures, the equilibrium gas phase concentration for the *same adsorbed VOC mass density* will be higher. This is considered in the model by multiplying the equilibrium relation with a ratio of saturation densities (5).

$$\rho_{g,eq}^{voc}(T) = \frac{\rho^{voc,s+g}}{K_{ma}} \frac{\rho_{g,sat}^{voc}(T)}{\rho_{g,sat}^{voc}(T_{ref})}$$
(5)

The key idea of the immobile-mobile phase model is, that the actual gas phase concentration may deviate from the equilibrium concentration. It will, however, in time approach the equilibrium concentration. This is modeled by defining the phase transition mass source/sink based on the difference between actual and equilibrium gas phase concentration (6).

$$\sigma_{g\to s}^{voc} = k_m \left( \rho_g^{voc} - \rho_{g,eq}^{voc}(T) \right) \tag{6}$$

When the actual gas phase concentration is higher than the equilibrium concentration, than some gaseous pollutants will be adsorbed. The  $\sigma_{g \to s}^{voc}$  is then positive and acts as a sink in the gas phase VOC balance equation, while acting like a source in the adsorbed VOC balance equation. The model is based on the observation, that the partition coefficient is obtained at 23 °C and thus indirectly includes the saturation density at 23°C. Using this model requires the saturation density of the VOC as function of temperature.

#### 5.1.5 Flux equations

#### Mass diffusion flux

Mass diffusion of VOCs is typically written in relation to a concentration gradient. However, from thermodynamics follows that the partial pressure gradient is the driving potential for gas diffusion processes<sup>46</sup>, which also includes the temperature effect. With increasing temperature, the partial pressure increases (related to the kinetic energy of the VOC molecules) and diffusion is accelerated.

The diffusive mass flux is proportional to the VOC permeability  $K_{voc}$  of the material (7).

$$j_{diff}^{voc} = -K_{voc} \frac{\partial p_{voc}}{\partial x}$$
(7)

$$j_{diff}^{voc} = -\frac{D_{voc,air}(T)}{\mu_{voc}R_{voc}T}\frac{\partial p_{voc}}{\partial x}$$
(8)

<sup>&</sup>lt;sup>46</sup> This can be derived from the gradient of chemical potential that appears in the Gibbs energy equation.

The permeability is proportional to the diffusion coefficient of the VOC in air  $D_{voc,air}$ , which is a temperaturedependent function. The tortuosity/pore structure of the material is incorporated in the diffusion resistance factor  $\mu_{voc}$  (8).

For a diffusion flux between two adjacent materials (or rather elements), the VOC permeability is averaged using a weighted, arithmetic average. If one of the materials is inert/tight for VOC diffusion, the flux is set to zero. See section 5.3.2 "VOC model settings", subsection "Material-material mapping" for details on material-VOC property mapping.

In case of isothermal conditions, the partial pressure gradient simplifies to a concentration gradient. First, the chain rule is applied since  $p_{voc}$  is a function of T and  $\rho_g^{voc}$  (see (4)).

$$\frac{\partial p_{voc}}{\partial x} = \underbrace{\rho_g^{voc} R_{voc} \frac{\partial T}{\partial x}}_{=0 \text{ in isothermal conditions}} + TR_{voc} \frac{\partial \rho_g^{voc}}{\partial x}$$

Then, the partial pressure gradient is replaced in (8), yielding the diffusion flux equation (9).

$$j_{diff}^{voc} = -\frac{D_{voc,air}\left(T\right)}{\mu_{voc}R_{voc}T}TR_{voc}\frac{\partial\rho_{g}^{voc}}{\partial x} = -\frac{D_{voc,air}\left(T\right)}{\mu_{voc}}\frac{\partial\rho_{g}^{voc}}{\partial x}$$
(9)

#### **Convective VOC transport**

When air/gas phase moves through the porous media, the VOC is transported alongside it. For a known gas mass flux  $v_{conv}^g$  the corresponding volumetric VOC flux is expressed simply by multiplication with the intrinsic gas phase VOC concentration  $\rho_e^{voc}$  (10).

$$j_{conv}^{voc} = \rho_g^{voc} v_{conv}^g \tag{10}$$

#### Boundary flux for VOC diffusion and for convective VOC flux

VOC diffusion across the boundary is described as driven by a difference in partial pressures between surface and outside air (11).

$$j_{diff}^{voc} = -\beta_{voc} \left( p_{voc,s} - p_{voc,e} \right) \tag{11}$$

However, to simplify use with established parameter sets, the boundary condition definition in DELPHIN requires a mass transfer coefficient  $h_{voc}$  to be provided, instead (see section 0). The mass transfer exchange coefficient  $\beta_{voc}$  can be computed from to the mass transfer coefficient  $h_{voc}$ , as described in section 5.2.4.

Convective VOC mass flux across the material boundary is described exactly the same as convective flux within the calculation domain.

#### Contact condition for VOC diffusion flux across material-air interfaces

When the calculation domain includes an air space (an air material, not a VOID), this material is identified by the AIR flag in the material file, and also when it is mapped to an Air material in the VOC database (see section 5.3.2). Instead of calculating the diffusion flux from a material to the air space via an averaged VOC permeability, the flux can be computed with a model that corresponds to the diffusion mass boundary flux (11).

The exchange coefficient is given, in this case, via a contact condition and overrides the calculation of the averaged permeability (see section 5.2.4 for information on how the mass transfer coefficient is converted into an exchange coefficient).

#### 5.1.6 Source/sink due to air change with ambient air

A field condition (source/sink) can be used to model air change with the ambient air. The air change rate due to mechanical ventilation  $n_{vent}$  is a model parameter. The model is applied to each selected element individually, resulting in a VOC source/sink  $\sigma_{vent}^{voc}$  (12).

$$\sigma_{vent}^{voc} = n_{vent} \left( \rho_{g,e}^{voc} - \rho_g^{voc} \right) \tag{12}$$

 $\sigma_{_{vent}}^{_{voc}}$  is positive, when the ambient VOC concentration  $ho_{_{g,e}}^{^{_{voc}}}$  is higher than the concentration in the element.

## 5.1.7 Calculation of diffusion resistance factor from model parameters

The mass diffusion equation (8) requires the VOC diffusion resistance factor  $\mu_{voc}$ . The VOC parameter database contains either the apparent diffusion coefficient D with respect to a gradient of the adsorbed VOC mass density  $C_m$  or the effective diffusion coefficient  $D_e$  with respect to a gradient of the intrinsic VOC mass density  $C_a$  in the gas phase (13).

$$j_{diff}^{voc} = -D \frac{\partial C_m}{\partial x} = -D_e \frac{\partial C_a}{\partial x}$$
(13)

Assuming local equilibrium and isothermal conditions, the flux equation can be rearranged.

$$j_{diff}^{voc} = -D \frac{\partial \rho_{g,eq}^{voc}(T_{ref})K_{ma}}{\partial x}$$
$$= -D \frac{\partial \frac{P_{voc,eq}}{R_{voc}T_{ref}}K_{ma}}{\partial x}$$
$$= -\frac{DK_{ma}}{R_{voc}T_{ref}}\frac{\partial p_{voc,eq}}{\partial x}$$

Through coefficient comparison we get an equation for the VOC diffusion resistance coefficient (14).

1

$$\frac{DK_m}{R_{voc}T_{ref}} = \frac{D_{voc,air}\left(T_{ref}\right)}{\mu_{voc}R_{voc}T_{ref}}$$

$$\mu_{voc} = \frac{D_{voc,air}\left(T_{ref}\right)}{DK_{ma}} = \frac{D_{voc,air}\left(T_{ref}\right)}{D_e}$$
(14)

#### 5.2 Parametrization of the model and VOC database

#### 5.2.1 Database file

The VOC and VOC - material parameters are stored in a VOC database file, usually with the extension ".vdb". The header file has the following structure:

```
# DELPHIN6 VOC Database File
# Lines beginning with a hash character '#' are comments and ignored
# Use the keyword 'undefined' for all string entries to indicate missing
information
# For constant "linear splines" simply store one x and one y value.
# Use -1e-100 for undefined/unknown values.
TABLE: VOC DATA
.... VOC parameter sets
TABLE: VOC MATERIAL DATA
.... VOC - material parameter sets
```

The first line is a comment and must contain the keyword DELPHIN6 to indicate that the new format for DELPHIN 6 is being used.

#### 5.2.2 VOC parameters

The VOC database defines basic properties of VOCs/pollutants. However, these properties are not needed for all balance equation combinations. The diffusion coefficient of the VOC in air  $D_{voc,air}$  must only be provided when air is being used in the construction. Otherwise, if the diffusion coefficient of air is not known, a value can be estimated ( $10^{-6}$  s<sup>2</sup>/m), since  $\mu_{voc}$  is computed from  $D_m$  first (see section 5.1.7). The same is true for the mass transfer coefficient  $M_{\rm w}$ .

For non-isothermal calculations, the saturation density of the VOCs must be provided as temperature dependent function. At least a single value must be given, in which case the temperature effect on the emission will be disabled.

The VOC parameters are specified in the VOC database, in table VOC DATA in the following format:

```
# ENTITY <string: VOC name>
#
   <string: alternative descriptive name(s)>
#
   <string: molecular formula>
#
   <string: source information, quality measure, reference>
#
   <double: molar weight in kg/mol>
#
   <double vec: temperatures for saturation densities in K> \,
```

- # <double vec: saturation densities in kg/m<sup>3</sup>(gas), one for each of the temperatures in the previous line>
- # <double vec: temperatures for diffusion coefficients in K>
- # <double vec: diffusion coefficients in air in m<sup>2</sup>/s, one for each of the temperatures in the previous line>

For example, the data entry for Formaldehyde looks like:

```
ENTITY Formaldehyde

50-00-0

CH20

Literature, ref. author and author2 (2011)

1083

253.15 258.15 263.15 268.15 273.15 278.15 283.15 288.15 ...

1.393 1.698 2.052 2.458 2.922 3.449 4.042 4.707 ...

296.15

1.455E-05
```

whereby Formaldehyde is the unique VOC identification name.

#### 5.2.3 VOC - material properties

For isothermal calculations the transport model requires only its diffusion coefficient with respect to the material  $D_m$  and the partition coefficient  $K_m$ . These are stored in the table VOC\_MATERIAL\_DATA, for combinations of a material and a VOC, in the following format:

```
# ENTITY
# <string:VOC name>
# <string:Material ID name>
# <string: source information, quality measure, reference>
# <double: diffusion coefficient D w.r.t material concentration in m<sup>2</sup>/s>
# <double: partition coefficient, K_ma in [m<sup>3</sup>(gas)/m<sup>3</sup>(REV)] >
```

Such an entry must exist for each material and VOC parameter set. There must not be an Air material in the database, since air materials are handled separately, already. The following example shows data for Particle board and Hexanal:

ENTITY

```
Hexanal
Particle Board
Literature, Deng et al. (2003), An analytical model for VOC emission from
dry building materials. Building and Environment.
7.65E-11
3289
```

The last line of this data block is optional and contains the water vapor diffusion resistance factor  $\mu$ . Since this value may not be available for all materials, it is indicated as *missing* by the special value -1e-100 in this example.

#### 5.2.4 Mass transfer exchange coefficient for diffusion boundary condition

The VOC diffusion mass flux across a boundary requires definition of a mass transfer coefficient  $h_{voc}$  with respect to differences in gas phase VOC concentrations. It is then converted to a VOC diffusion exchange coefficient as follows:

$$j_{diff}^{voc} = h_{voc} (\rho_{g,s}^{voc} - \rho_{g,e}^{voc})$$
$$= \frac{h_{voc}}{R_{voc}T} (p_{voc,s} - p_{voc,e})$$

Comparing coefficients gives an equation for the mass diffusion exchange coefficient (15).

$$\beta_{voc} = \frac{h_{voc}}{R_{voc}T}$$
(15)

# 5.3 Definition of VOC models in the DELPHIN 6 user interface

### 5.3.1 Enabling pollutant balance equation

Open the simulation model view and check the respective balance equations, as shown in Figure 42 for the balance equation combination HAP.

The corresponding balance equation keywords in the project file are: BEPollutant, BEHeatPollutant, BEAirPollutant, BEHeatAirPollutant

Senergy Balance Equation		
Default initial temperature:	20	С
<ul> <li>Use thermal conductivity of dry material (LAMBDA)</li> </ul>		
$^{\odot}$ Use design value of thermal conductivity (LAMBDA_DESIGN)		
○ Use moisture-dependent thermal conductivity		
Default initial relative humidity:	80	%
Moisture Balance Equation		
Default initial relative humidity:	80 %	6
Use Kirchhoff potential for liquid flux calculation		
Use gravity		
Use equilibrium ice model		
Air Mass Balance Equation		
Use gravity		
Salt Balance Equations		
Salt Simulation Options		
Pollutant Balance Equations		
VOC Simulation Options		

Figure 42: Screenshot of the Simulation Model Options in DELPHIN 6, with energy and pollutant balances and quasisteady air flow model enabled

#### 5.3.2 VOC model settings

#### Selection of VOC database and VOC to be calculated

Once the pollutant balance equation has been enabled, the button to open the VOC simulation options is enabled. Pressing this button opens the dialog shown in Figure 43.

In the dialog, first a VOC database file has to be selected. Once the database file has been chosen, it will be automatically read. Alternatively, or in case of database errors, you can click on "Update list from database", to refresh the VOC data table.

Next, select the row with the VOC to be used for calculation.

Lastly, specify the DELPHIN 6 material to VOC DB material mapping as described below.

The VOC modeling data is store in the project file in the following XML block within the Init section:

```
<ModelSettingsVOC>
```

```
<VOCDatabase>/tmp/demonstration/VOCEmissionTest/voc_data.vdb</VOCDatabase>
<VOCID>Hexanal</VOCID>
<MaterialMapping>Air gap 50 mm (vertical) [18] == Air</MaterialMapping>
<MaterialMapping>Particle board [348] == Particle Board</materialMapping>
```

```
</ModelSettingsVOC>
```

ata base								
Pollutant data base: /home/ghorwin/svn/Delphin6_trunk/data/demonstration/VOCEmissionTest/voc_data.vdb Import								
Reference:	/home/ghorwin/svn/Delp	hin6_trunk/data/demonstratior	n/VOCEmissi	onTest/voc_data	.vdb		Edit.	
	<ul> <li>Reference with file path relative to project file</li> </ul>							
	Paferance with file path relative to installation directory							
		the file asth	UI y					
	Reference with absolution	ite file path						
OC/pollutant seled	tion							
Update list from (	database							
VOCs/Pollutants (g	gaseous components):							
Name	Desc	ription	Formula	Molecular M	ass [g/mol]	Liquid dens	ity [kg/m3]	
Cyclohexane	110-82-7	C	5H12		0.0842		770	
Decane	124-18-5	C	10H22	0.1420			735	
Dodecane	112-40-3	C	12H26	0.1700			753	
Ethylbenzene	100-41-4	C	3H10	0.1060			867	
Formaldehyde	50-00-0	CI	120	0.0300			1083	
Heptanal	111-71-7	C	7H14O	0.1140			818	
Heptane	142-82-5	C	7H16		0.1000		684	
Hexanal	66-25-1	C	5H12O	0.1000			818	
Limonopo	120-06-3	C	0.1360			010		
(+(				)			UNIT	
Database contains aterial mapping	29 VOCs and 15 materials.							
Database contains aterial mapping Material file/r	29 VOCs and 15 materials.	Material ID in VOC database	Partition	Coefficient (Km)	Diffusion Coe	efficient (Dm)		
Database contains aterial mapping Material file/r 1 Particle board [	29 VOCs and 15 materials. reference in current project [348]	Material ID in VOC database Particle Board	Partition ( 3289	Coefficient (Km)	Diffusion Coe 7.65e-11	fficient (Dm)		

Figure 43: VOC/pollutant model settings; selection of database file, selection of VOC to be calculated, and materialmaterial mapping

### Material-material mapping

The VOC database is maintained independently of the DELPHIN 6 database. Also, materials that are tested for VOCs are often not tested for moisture transport and storage parameters. Therefore, the materials in the VOC database may not correspond to materials from the DELPHIN 6 database.

The VOC model settings dialog allows to assign specific VOC - material database materials to materials used in the DELPHIN project. In the table, the first column lists the material reference names of all materials used in the project (mind, also unused materials are shown here). The second column can be edited and a material used in the VOC database can be selected. The list of available materials includes only those materials that appear in dataset defined for the combination of the material and the currently selected VOC.

Therefore, changing the current VOC in the database may require re-mapping materials!

In addition to parametrized VOC/materials combinations, an *Air* material and an *Inert/VOC-tight* material is offered for mapping. These special cases are interpreted as follows:

- Air materials only hold gas phase VOCs (no adsorbed phase) and a partition coefficient and material diffusion coefficient is not required
- Inert/VOC-tight materials do not contain VOCs; fluxes and source are ignored for such materials

## **Defining initial conditions**

Initial concentration of VOCs are defined via initial conditions. Hereby, the initial adsorbed VOC concentration  $C_{m0}$  is defined and assigned to the element range of interest (default method as for custom temperature/moisture conditions). VOC initial conditions are of type VOCMass.

#### Defining air change rates

When simulation chamber tests, the air volume elements beside the VOC emitting material receive a field condition of type AirChange.

#### VOC related boundary conditions

Generally, the engineering interfaces do not consider VOC diffusion, hence surfaces with plain engineering interfaces are tight with respect to VOCs. If VOC transfer shall be permitted, a DETAILED interface type has to be used and VOC related boundary conditions have to be specified manually.

#### VOC diffusion boundary condition

A boundary condition of type VOCDiffusion can be defined to model VOC emission from a material surface. The only parameter expected is the mass transfer coefficient  $h_{voc}$  of the VOC with respect to the gas phase VOC concentration and given at  $T_{ref} = 23^{\circ}C$ . According to equation (15), the exchange coefficient with respect to partial pressure of the VOC is then:

$$\beta_{voc} = \frac{h_{voc}}{R_{voc}T_{ref}}$$

Currently, this transfer coefficient is kept constant in the model regardless of the surface/air temperature.

## 5.4 Review and definition of similarity factors

#### 5.4.1 Diffusion similarity factor

Emission analysis includes VOC transport and storage in porous materials. Beside several material and VOC parameters, there are two decisive parameters, which depend on materials and VOCs: the apparent diffusion coefficient  $D_m$  and the partition coefficient  $K_{ma}$ . The apparent diffusion coefficient is related to the absorbed VOC concentration gradient in the material, while the effective diffusion coefficient, given by  $D_e = D_m \cdot K_{ma}$ , is related to the VOC concentration gradient in the gaseous phase of the material. For non-isothermal conditions, the effective diffusion coefficient must be related to the partial pressure gradient.

There is not much data on diffusion and partition coefficients. Therefore, similarity variables have been introduced to predict these coefficients from moisture measurements. In building physics, the water vapor diffusion resistance factor  $\mu_{vap} = D_{e,vap}^{air} / D_{e,vap}^{mat}$  is used to capture the effects caused by the material's porosity and tortuosity. It relates the effective diffusion coefficient of water vapor in air to the one in the porous material. Similarly, a VOC diffusion resistance factor  $\mu_{voc} = D_{e,voc}^{air} / D_{e,voc}^{mat}$  can be introduced. Then, the diffusion similarity factor is given by

$$\kappa_{diff,voc} = \frac{\mu_{voc}}{\mu_{vap}}$$
 Diffusion similarity factor. (16)

The diffusion similarity factor  $\kappa_{diff,voc}$  depends on material properties and VOC properties. In the following section 5.6, there will be an analysis of the calculated diffusion similarity factors in relation to available VOC properties. It is possible to predict VOC diffusion resistance factors (for a different VOC but the same material) on the basis of these relations.

#### 5.4.2 Partition similarity factor

The moisture absorption in porous materials is described by sorption isotherms  $\theta_l(RH)$ , which relates the moisture content  $\theta_l$  to the relative humidity RH at constant reference temperature  $T_{ref}$ . A schematic curve of a sorption isotherm is displayed in Figure 44. Water vapor diffusion measurements are done by the so-called "Dry Cup" and "Wet Cup" experiments. For both experiments, which yield  $\mu_{vap} = \in [\mu_{dry}, \mu_{wet}]$ , a mean relative humidity in the sample can be determined.

The slope of the sorption curve (at constant temperature) is the specific moisture capacity,  $\xi$ ,  $m^{3}_{H20}/m^{3}_{mat}$ , at a given relative humidity.

$$\xi = \frac{\partial \theta_l}{\partial RH}$$
 Specific moisture capacity. (17)



Figure 44: Schematic sorption isotherm with definition of two moisture capacities.

As shown in Figure 44, the mean relative humidity of "Dry Cup" and "Wet Cup" experiments can be used to define two partition coefficients of water vapor.

$$K_{ma,H2O,dry} = \frac{\rho_l R_{vap} T_{ref}}{p_s(T_{ref})} \cdot \zeta_{H2O,dry}$$
(18)

$$K_{ma,H2O,wet} = \frac{\rho_l R_{vap} T_{ref}}{p_{sat}(T_{ref})} \cdot \zeta_{H2O,wet}$$
(19)

The first steep range from RH = 0 to about 20% RH may be most appropriate to serve as a proxy for VOCsorption, since VOCs typically deposit in monolayers, like the initial low-RH sorption of water vapour. Therfore,  $K_{ma,H2O,dry}$  is used to introduce a partition similarity factor.

$$\kappa_{part,voc} = \frac{K_{ma,H2O,dry}}{K_{ma,voc}}$$
 Partition similarity factor. (20)

The partition similarity factor  $\kappa_{part,voc}$  depends on material properties and VOC properties. In future, there should be an analysis of the calculated partition similarity factors in relation to available VOC properties. It would be possible to predict partition coefficients (for a different VOC but the same material) if sufficient relationships can be found.

## 5.5 Evaluation of CHAMPS-BES data and diffusion coefficients from literature

From preliminary investigations, the hypothesis was established that the diffusion similarity factor should depend on the physical / chemical properties of the VOC molecules. Evaluation of the VOC database content of the CHAMPS-BES software shows that it decreases linearly with the decadal logarithm of the partition coefficient (Figure 45). It can be concluded that higher partition coefficients correspond with higher VOC concentrations absorbed by the material, i.e. the apparent diffusion resistance decreases with higher VOC concentration due to diffusion "shortcuts" created by absorbed VOC islands.



Figure 45: Analysis of the VOC database content of the CHAMPS-BES software.

Using data from (Liu, Nicolai, Abadie, Qin, & Zhang, 2018), which was provided as part of the Annex 68 ST2 work, apparent diffusion coefficients  $D_m$  and partition coefficients  $K_{ma}$  with respective references could be analyzed for different VOC / material combinations. The data includes measurements from (Xu, 2012) who measured VOC and water vapor diffusion flux at identical material samples made from Calcium silicate.

In a first step, all material / VOC combinations were plotted together in one graphic, which led to a large scatter as displayed in Figure 46. Neverthelless, first conclusions can be drawn: It became clear that the data should be separately analyzed for each material and data should be represented in log<sub>10</sub> scales in order to see effects.



Figure 46: Graphical visualization of VOC-material data given by Zhenlei Liu et al. The log<sub>10</sub> data of the diffusion resistance factor and the diffusion similarity factor is plotted against the log<sub>10</sub> data of the partition coefficient. No trend can be recognized since all material / VOC combinations are displayed.

# 5.6 Establishment of diffusion similarity relations

Figure 47 shows how VOC diffusion coefficients in air vary with molar mass of the VOC. The analysis of the VOC diffusion coefficients in the CHAMPS-BES database revealed that all data points follow a natural logarithm law. The diffusion speed at given pressure difference decreases with higher molar mass.



Figure 47: Diffusion coefficients of VOCs (blue) and water vapor (red) in air at 23°C as function of molar mass

With the trend equation displayed in Figure 47, one source of uncertainty can excluded in further calculations. The further data analysis calculation comprises the following steps:

- 1. Calculation of the effective diffusion coefficient  $D_e = D_m \cdot K_{ma}$
- 2. Calculation of the diffusion resistance factor  $\mu_{vac} = D_e^{air} (23^{\circ}C)/D_e$  by using the trend eq. above
- 3. Calculation of the diffusion similarity factor  $\kappa_{diff,voc} = \mu_{voc} / \mu_{dry}$  by using the dry cup value

In order to get the correct water vapor resistance factors  $\mu_{dry}$  (step 3), the respective material used for VOC measurements must be identified in the material database of DELPHIN6. The dual chamber experiment, reported by (Xu, 2012), was carried out for water vapor and six different VOCs. Some of the measurements were replicated. A  $\mu_{dry}$ -value of 8.75 was reported which is in good agreement with the cluster average of 6.5. The  $\mu_{voc}$ -values are in the same order of magnitude (1.5-4.5). The analysis of Calcium silicate data supports the initially supposed trend (Figure 48): the diffusion similarity factor decreases with higher partition coefficients.

Except for Calcium silicate, the materials were just referenced by name, which makes their identification very complicated. Since no further material parameters are provided along with the materials, the water vapor diffusion resistance factors must be regarded as uncertain quantity. In future, some additional building physical properties should be measured along with the VOC diffusion experiments. This would greatly help to identify the correct material to derive the respective water vapor resistance factor.

In order to avoid the problem in the short term, all materials were collected in the DELPHIN6 database with names that indicate similar material types, and cluster mean values were defined, which were used as initial

estimates for the  $\mu_{dy}$ -values. This leaves an inherent uncertainty that leads to a possible vertical shift of the similarity factor.

Figure 48 shows that all materials analyses support the initially supposed trend indicated in Figure 45. It can be concluded that the diffusion similarity factor systematically decreases with higher partition coefficients. Since each trend curve represents a different material, it follows that the slope of the curves depends on certain material properties. Until now, it has not been investigated, which material property could be used to predict the slope of the diffusion similarity factor function.



Figure 48: Diffusion similarity factors of analyzed materials

# 5.7 Continuation of the 2D Common exercise: DELPHIN6 VOC test cases

In order to test the derived similarity relations and the new VOC model, as well as their implementation in DELPHIN6, a series of tests was created, which continues the 2D common exercise with the PASSYS cell. For this purpose, an initial concentration of 30000 mg/m<sup>3</sup> Hexanal was introduced into the floor plate of the test room in order to simulate the emission from the material into the indoor air of the test room. The 3 mm steel coating of the base board has been removed so that the PS foam is in direct contact with the air and the VOC can be emitted.

Following cases were compared:

- 1) Air exchange vs. airtight construction
- 2) isothermal vs. non-isothermal conditions.

The effects to be examined here are both the temporal course of the emission rate and its temperature dependence. The emission rate is expected to increase with temperature. In the case of airtight construction, the Hexanal 's mass conservation is also checked.

## 5.7.1 Pollutant emission from a material under isothermal conditions

The construction setup of the PASSYS cell for isothermal test case is shown in Figure 49. The full size 2D model of the PASSYS cell from the common exercise is used for this purpose. In the isothermal case, only the VOC mass balance is solved and no boundary conditions are assigned to the cell, i.e. thermal flux is not calculated and the VOC flux at the external surface is zero. The constant reference temperature for calculation of thermodynamic properties of the VOC is 23°C.



Figure 49: Construction setup of the PASSYS cell for the isothermal test case

The pollutant source results from the initial condition of the PS board in the floor of the test room. The emission of the Hexanal increases the VOC concentration in the air of the test room over time. A duration of 20 days was set to investigate this process with and without air change in the test room. Without air change (ACH = 0 h<sup>-1</sup>), the expected equilibrium concentration in the room air is close to 10 mg/m<sup>3</sup>, since the initial condition is 10 times higher than the partition coefficient of the material, which is 3000. With air change (ACH =  $0.2 h^{-1}$ ), the equilibrium concentration in the room air must be lower, since it is assumed that there is no VOC in the outside air. In addition, a different distribution of VOC in the test room air volume is expected for these two cases. The entire VOC mass balance has been verified and validated for all cases.

The course of the VOC concentration in the test room air and the respective VOC concentration fields are shown in Figure 50 and Figure 51. As can be seen, the temporal course of the emission meets the expectations in both cases. The graphs show a time series of VOC concentration fields at t = 0.5, 3, 10 and 19 d. At the beginning the fields with and without air exchange look very similar. Over time, the room air is kept cleaner with air exchange, as expected. Only in the immediate vicinity of the ground floor a higher VOC concentration can be observed.

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Figure 50: Temporal courses of the VOC concentration in the room air of the test room of the PASSYS cell without (left) and with air change (right), the time points of the following field snapshots are indicated by the vertical lines.



Figure 51: Snapshots of the VOC concentration field in the room air and in the gas phase of the floor panel without (left) and with air change (right) after 0.5 / 3 / 10 and 19 days.

## 5.7.2 Pollutant emission from a material under non-isothermal conditions

The construction setup of the PASSYS cell for non-isothermal test case is shown in Figure 52. The difference is a thermal boundary condition with an external air temperature of 20°C and ground temperatures of 0, 20 and 40°C. Of course, a ground temperature of 40°C is exceptionally high and may be unrealistic, but this is an academic test case to accelerate the emission from the material. In turn, 0°C ground temperature should delay the emission. As in the isothermal test case, the cases are compared with and without air change.



Figure 52: Construction setup of the PASSYS cell for the non-isothermal test case

As shown in Figure 53, there is a clear temperature effect: higher temperatures generate larger emission rates and higher equilibrium concentrations in the room air. The results are consistent with the experimental results. The effects can be traced back to the balance equation model for VOCs implemented in DELPHIN6 that contains a phase transition term that communicates between the mass balances in the gas phase and the absorbed phase. The key idea of the immobile-mobile phase model is, that the actual gas phase concentration may deviate from the temperature dependent equilibrium concentration. It will, however, in time approach the equilibrium concentration. This is modelled by defining the phase transition mass source/sink based on the difference between actual and equilibrium gas phase concentration.

The results are consistent with the previous isothermal case: the reference temperature 23°C-curves lie slightly above the non-isothermal 20°C-curves. In addition, Figure 53 shows the temperature fields after 20 d for both 0°C and 40°C ground temperatures. It can be seen that the air change with 20°C external air temperature has the expected impact on the room air temperatures.

In summary, the tests provided insight into the capabilities of the new VOC model implemented in DELPHIN6. All tests were successful and the results were in line with expectations. Other features may be required, such as the implementation of a time-dependent VOC sink or source, which may be applied, for example, in indoor air. In addition, complete coupling to the hygrothermal simulation is not yet realized and the airflow network cannot be used together with the VOC mass balance.

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temperature fields for 0°C and 40°C ground temperature at t=20 d (middle and bottom left and right)

# 6 Quality assurance protocols and standards

The recent past has shown, that the importance of simulation tools in the fields of planning and operating buildings and districts has increased massively. Especially highly ambitious and innovative systems require detailed simulation to achieve a proper understanding of the systems dynamic and therefore allow an appropriate system design. This technical necessity has already been addressed by lawmakers, allowing to use simulation-based analysis rather than classic procedures using normative calculation methods.

With the ongoing penetration of simulation software into the planning process, it gets more and more important to improve the comparability and transparency of simulation models along the overall simulation tool developments. So far, validation and certification are almost always up to the software developer and cannot be reproduced by third parties. This is particularly problematic since the quality of the conclusions that can be drawn from simulation results highly depends on the quality of the simulation itself.

In order to tackle the abovementioned problems, the German Federal Ministry for Economic Affairs and Energy currently financially supports the **SimQuality** project (03ET1570A-G) "Development of quality standards for building and quarter energy performance simulation as a planning tool". The project runs from August 2018 until July 2021. In accordance with the Annex 68 ST3 common exercise, selected simulation tools as shown Table 17 are used to solve common exercises.

Name of the software tool	Developer / License holder
THERAKLES / NANDRAD	Institute of Building Climatology, Dresden, Germany
Building Simulation	Hottgenroth Software GmbH, Cologne, Germany
EnergyPlus	Department of Energy (US)
IDA ICE	EQUA Simulation AB
TRNSYS	TRANSSOLAR
Building models and libraries from EBC Annex 60	e.g. AixLib (Modelica), RWTH Aachen, Germany

#### Table 17: Overview of the software tools used in the SimQuality project

The SimQuality participants come from research institutes (TU Dresden, RWTH Aachen, University of Applied Sciences Munich), planning firms (Innius DÖ GmbH Dresden and Planungsgruppe M+M AG) and software industry (Hottgenroth Software GmbH & Co. KG). Among others, the goal of this project is to define quality standards for simulation software, hereby developing a validation methodology based on individual validation cases. Further, it is anticipated to compile guidelines for new simulation users and suggestions for further development of norms in this field. Comparing simulations tools and investigating model errors regarding practical test cases might yield new findings.

# 6.1 A different approach to continue the common exercises

The task of the common exercises executed within the scope of Annex 68 was to define and develop test cases in order to compare different simulation tools with a focus on investigating individual physical effects. This is the academic approach of defining test cases to identify and quantify model errors and it represents the software developers perspective.

In contrast to this, the aim of the **SimQuality-Project** is to complement this approach by the practical perspective. Therefore, planning firms were invited to participate in the project. The new target is to extract relevant models and the corresponding model specifications from practical applications from the planning process.

In comparison to the developed test cases in this report, the test cases derived from the planning practice might especially vary in size and complexity of both the geometry and the technical systems. Therefore, the test cases will be restricted to just one geometry as the PASSYS cell in the Annex 68 common exercises.

# 6.2 The SimQuality workplan

In future, simulation methods will be used in planning practice for a wide variety of application scenarios. To test correct evaluation of such problems with the use of simulation software programs, a testing procedure for such simulation programs is envisioned. Hereby, realistic application scenarios are modeled in different levels of complexity. The practical complex applications are translated into testable individual problems (validation cases), in order to analyze and quantify different sources of errors separately and to avoid overlapping effects and misinterpretations. The content and the sequence of the validation cases are coordinated with the practice partners to take into account their requirements in particular.

Validation cases map application scenarios with different physical complexity and specify the parameterization of specific partial problems. Each case is supplemented by a description of the internal and external boundary conditions, and other model parameters. Further, rules for analysis and interpretation of calculation results are specified. Hence, the results of individual test cases can be compared among different simulation programs and results can be classified via suitable comparison methods (e.g. band of acceptance).

The validation cases are designed such that the model complexity builds up successively. Meaningful levels of complexity of the validation cases have to be defined by the research partners to ensure the diagnostic capability of the methodology. In addition, the existing validation cases from national and international standardization and scientific sources are analyzed, systematized and extended to include the uncovered cases. The work plan depicted in Figure 54 reflects this approach.

A reference solution specifies the range of solutions within realistic accuracy tolerances. A validated planning tool that meets the quality criteria must be able to reproduce this reference solution within the error range limits. The planned validation procedure is divided into the following steps:

- 1. In the first step, analytical solutions for highly simplified validation cases are given. Simplified validation cases with analytical solutions have to be reproduced to the present standards of numerical methods with very high accuracy. Greater deviations from analytical and numerical solution indicate poor implementation of the mathematical solution methods (e.g., discretization, time stepping control). Such defects must be improved.
- 2. Based on this, validation cases with increasing physical complexity and dynamics are defined. For such cases, there are no analytical comparative solutions and it must be decided according to plausibility and exclusion principles, which solution is recognized as correct. A correct solution can be found, for example, if the vast majority of established programs agree (comparative validation). Alternatively, e.g. also measurements under defined laboratory conditions possible (empirical validation). The range of possibilities is naturally greater with complex physical problems. If a procedure is too far out

of range, the source of the error (implementation error, too simplified model, misinterpretation of parameters, etc.), needs to be identified and, if possible, eliminated.

3. Very complex validation cases involving different producers, consumers and load profiles may mean that they cannot be mapped by the majority of models. Too much scatter of the results then calls into question the determination of a correct solution. One possibility would be to define solution corridors / fronts. In such cases research needs are identified that are also of interest to the model developers. In practice, this means that there is not yet a sufficiently tested solution available. By pointing out the limits of the application possibilities of simulation methods, uncertainties in planning practice can be reduced.



Figure 54: SimQuality work packages

The use of simulation programs enables the consideration of location and climate-specific parameters in high temporal resolution. There is no need to introduce lump sums, as is common with hand-held computing methods. This will improve the conditions for harmonizing reference solutions at European or international level.

In the future, quality assurance should lead to bringing developments from science into practice more quickly. The elaborated validation cases, usage scenarios, climate models and reference solutions shall be made publicly accessible in cooperation with the accompanying research of the research network. In the future, simulation models with quality certificates that cover a range of use cases will be made available on a central data and model platform.

# 6.3 The SimQuality platform

The **SimQuality-Platform** will allow external users to define and describe their own test cases and allow different parties (for example: software-developers, institutes ...) to recreate the simulation results. To make these results accessible to the public, the **SimQuality-Platform** is developed as an interactive web tool. On the one hand, this website is supposed to provide public access to project results from the SimQuality project.

On the other hand, the website will make it possible for every software developer to participate in the workflow and upload their own simulation results and test it against other simulation tools. Also, all the uploaded simulation results and simulation models will be clearly represented are available for download.

The selected approach for simulation software quality assurance is to compare the simulation results for predefined Use Cases run by various simulation tools, different versions and by different users. If the simulation results between all these variations is identical/very similar or at least within an acceptable range, it can be assumed that the simulation results and therefore the used tools are correct. This method of "cross-validation" is already used in different projects.



### Figure 55: Screenshot of the prototype of the SimQuality-Platform

Figure 55 shows a screenshot of the current stage of the SimQuality-Platform prototype. The menu bar on the left is used to navigate between Use Cases. For the sake of better overview, the Use Cases are divided into different categories where each category also provides an overview section. Once the user chooses a Use Case, for example the calculation of the solar position, the website will redirect to the specific Use Case page.

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Here the user will find a detailed explanation of the Use Case itself and further meta-information about the simulation results.

After that the desired simulation results need to be chosen. The table contains all the stored simulation results, clearly represented by the general information (author, software, version ...) as well as the Use Case-specific variations such as the city and the day in the context of the above-mentioned calculation of the solar position.

Below this table, the results of the present Use Case for all the selected variations are shown. In order to further investigate differences, it is possible to interactively zoom and move the timeline. The available graphical interface will differ between the different Use Cases in order to provide the best usability and clearest representation for every specific Use Case.

The SimQuality-Platform is still under development and will be available by the end of 2020.

# 7 Conclusions and outlook

Major findings from subtask 3 can be summarized as follows:

- There is a significant knowledge gap in integrating modeling and simulation tools developed for different purposes such as energy performance, IAQ and life-cycle cost analysis. The Modelica and CHAMPS simulation platforms assisted with the functional mock-up interface technique for cosimulation present a viable approach to the integration, and hence should be further developed.
- 2) There is also a significant gap between simulation tools for research and those needed for practice in the industry. Simplified simulation model and easy-to-use platform while providing reliable building performance predictions are essential. Criteria on and balance between required accuracy and acceptable calculation speed of building performance simulations need to be established for various building plan, design, and operation stages. A standard protocol for quality assurance of the modeling and simulation results needs to be developed. The SimQuality platform offers an opportunity and viable approach for the development through multi-national collaboration.
- 3) A series of simulation cases for common exercises from simple to increasingly complicated scenarios have been established to enable comparisons of different simulation tools and identify their limitations. They can be further used to evaluate new models or simplified simulation tools for practical applications.
- 4) Limited input data regarding pollutant transport and storage properties of building materials continue to be a barrier for wide application of CHAMPS and other simulation tools for indoor air quality analysis. The similarity theory between the VOC and moisture transfer in porous media has been further developed in this study, including a proposed approach to estimate the VOC sorption characteristics from the moisture sorption isotherm of the material as well as similarity in diffusion resistance previously established. Experimental data are needed to further develop and validate the similarity theory, which would enable the establishment of a database of VOC transport and storage properties of various building materials for indoor pollution load and IAQ analysis similar to the heating/cooling load and hygrothermal performance analysis.

Future planning tools must deliver high quality results based on high quality input data; a task that has to be secured by better quality standards. The new quality standards to be developed relate, among other things, to the scientifically sound quality of the physical models, the validation level of the models and input data, the accuracy and efficiency of the mathematical solution methods, the ability to network with other tools, the integration of building information models and the traceability and verifiability of the results. A practical way to implement quality assurance is to define publicly available reference solutions. Since there are a multitude of application scenarios (components, buildings, quarters, etc.), a publicly funded test suite of individually tailored reference solutions with characteristic test cases would be useful for the validation of commercially distributed planning tools.

The required measures are to be implemented in cooperative work of partners from science and practice. To empower users to cost-effectively exploit optimization potential, high-quality mathematical and physical processes must be paired with ease-of-use and processing efficiency. The calculation results of the planning tools are to be prepared for the efficient decision-making and certification. To support the acceptance of modern planning tools, publicly funded monitoring projects must provide big data available in publicly

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available databases. This generates new knowledge - for example, about user behavior - which helps to tap further savings potential.

Huge intelligence and financial resources have been invested in creating simulation codes and tools. However, most existing building simulation tools remain at the research or "in-house" level and are not widely used in construction practice. The main tasks of the CHAMPS platform are to promote the practice integration of simulation tools and to facilitate complex practical planning tasks by supporting interdisciplinary teamwork.

An increased use of simulation tools has already been observed in practice. This goes hand in hand with the general trend of digitization of our society and in particular of the construction sector. The responsibility of researchers in technical fields such as building physics and indoor air quality today is not just to provide good research results. They are also responsible for the transfer of knowledge, which means that the usability of the research results must be ensured. This is only possible if the researchers themselves are also working on practical projects to see where the weak points of their tools are and how to improve them.

It is not uncommon for researchers to shoot beyond the target during development. The direct feedback with the practice can help to avoid the implementation of unnecessary functions. The increasing practice integration helps, as the example of the CHAMPS platform demonstrates, to formulate research questions in a more precise and practical way. Digitalization in construction thus contributes to improving resource efficiency.

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# **Appendix 1: 2D Simulation results**

# **Overview of variants**

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# Encoding

The variants are coded according to the following scheme: PASSYS-2D-HHH-Wall-size-air-rain

PASSYS	Base construction to be simulated, the PASSYS cell
2D	Dimensions of the problem, in this exercise always 2D
ННН	Considered mass and energy flows (H = Heat, A = Air, M = Moisture)
Wall	Base material of the exchangeable west wall (= PSBoard or Brick), mortar joints are neglected
size	Size of the PASSYS cell (= <u>normal</u> , small and verysmall) - normal is the default case
air	Air flow handling (= <u>noair</u> , airchange, airgap) - noair is the default case
rain	Rain load handling (= norain, <u>rain)</u> - rain is the default case

# 1 PASSYS-2D-H-PSBoard: External long-wave and short-wave radiation

# **1.1 Construction**

The normal-size PASSYS cell used in this variant (Figure 1) has the same dimensions as described in Chapter 4 of this report. The construction is as simple as possible; all unnecessary details have been neglected. The basic construction consists only of metal-coated PS foam panels for flat roof, floor and west wall, which are stabilized with H-steel girders. The test room is installed with interchangeable partition and east wall and additional insulation elements on the ceiling and floor. No support structure is considered in this common exercise.



Figure 1: Discretized normal-size PASSYS cell (all dimensions are internal dimensions). The lightweight basic construction consists of 100 mm metal-coated PS foam panels, while the test room was installed with 300 mm panels. 100 x 100 H-Steel beams (9 mm) stabilize the construction, but form thermal bridges.

# 1.2 Modeling assumptions and parameter settings

In this first variant, only the energy balance equation is solved, no moisture effects are taken into account. No momentum balance equation is taken into consideration for the zone air. Instead, the thermal effects of air movement are approximated by increased thermal conductivity of the air.

A free-running building is modeled, i.e. no operation of HVAC devices is considered. The building is only influenced by its ambient environment, taking into account the heat transfer through walls and the long-wave and short-wave radiation from outside to the east / west walls and the flat roof. In particular, the processes listed below are taken into account:

- Heat convection /conduction between room zone , constructions and external air
- Heat storage in construction elements and inside zone air
- Heat transport in inside zone air
- Heat transport between floor and ground

• Short-wave and long-wave radiation on external construction surfaces

The thermal material parameters are listed in Table 1. CHAMPS-BES, DELPHIN5 and DELPHIN6 treat the zone air as "special material" with the parameters also shown in Table 1.

	Thermal conductivity In W/mK	Bulk density In kg/m³	Specific heat capacity In J/kgK
Steel	20	8000	920
PSFoam-expanded	0.04	34	1300
Zone air at 20°C	0.27	1.205	1000

### Table 1: Material parameters of Metal, PS-Foam and Zone air

Heat convection and shortwave and longwave radiation are considered for external surface of roof, east and west walls.

Constant convective heat transfer coefficients are used for heat convection calculation. The external and internal wall structure convective heat transfer coefficient are assumed to be 25 W/m<sup>2</sup>K and 8 W/m<sup>2</sup>K, respectively. Absorption coefficient of building surface is 0.6, reflection coefficient of surrounding ground is 0.2 and emission coefficient of building surface is 0.9.

The ground temperature is constant at 8°C all year round. The convective heat transfer coefficient between ground and floor is set at 1000 W/m<sup>2</sup>K, which imposes a Dirichlet boundary condition. The initial temperature is 5°C. The simulation starts on January 1<sup>st</sup> and the entire simulation duration is 365 days.

# **1.3 Simulation results**

The output variables are written at predefined output times in data files that have been set differently for field outputs (2.5 daily) and single value outputs (1 hourly).



Figure 2: Temperature fields at Jan-6-0:00, Feb-2-12:00, Apr-3-12:00, Jul-20-0:00 after 5, 32.5, 92.5 and 200 days

The temporal change in the temperature fields, which show the influence of the boundary conditions and the thermal bridges, is shown in Figure 2 for three successive times. Blue colors indicate cold and red colors warm temperatures. For example, February 2 stands for a cold day and April 3 for a warm day. In both cases, the temperature fields are displayed at 12:00 p.m. The annual and daily temperature amplitudes should increase with less insulation and less buffer capacity. As shown in Figure 3 and Figure 4, this can be clearly demonstrated by the temporal course of the temperatures in the test room, service room, internal surface east wall, middle position east wall and external surface east wall.

The temperature curves of the other walls, roof and floor show the same trend. In summary, all results meet expectations. The tested programs CHAMPS-BES, DELPHIN5 and DELPHIN6 deliver identical results for this variant. The different curves cannot be distinguished with the naked eye.



Figure 3: Comparison of test room (above) and service room (below) air temperatures



Figure 4: Comparison internal (above), middle (middle) and external (below) east wall temperatures

### Appendix 1

# 2 PASSYS-2D-HM-PSBoard: Moisture fluctuation in rooms

# 2.1 Differences to the previous variant

The moisture mass balance is added and solved together with the energy balance. Since the construction is completely moisture-proof, no moisture can be exchanged with the external environment, i.e. the moisture balance only affects the room air. All other settings remain unchanged.

# 2.2 Construction

The normal-size PASSYS cell is used - see section 1.1.

# 2.3 Modeling assumptions and parameter settings

Basic moisture related parameters are listed in Table 2. For more information such as vapor conductivity function, moisture retention curve, and liquid water transport function please refer to the DELPHIN5 or DELPHIN6 materials database.

	Open porosity in m³/m³	Effective saturation in m <sup>3</sup> /m <sup>3</sup>	Water vapor diffusion resistance factor in -
Steel	1e-05	1e-06	1e+11
PSFoam-expanded	0.94	0.935	96
Zone air at 20°C	1	1	0.3

### Table 2: Hygric material parameters

The moisture boundary condition (humidity + rain + wind) and moisture buffering in the walls should have no effect since the construction is moisture-proof. This can be achieved by omitting the hygric boundary conditions, whereby the flow is set to zero. In this variant, however, the hygric boundary conditions of the construction were assigned to test whether CHAMPS-BES, DELHIN5 and DELPHIN6 ignore any moisture flow in moisture-resistant constructions.

# 2.4 Simulation results

Since this variant uses a moisture-proof construction, the zone moisture mass must remain constant, as shown in Figure 5.

The coupling between heat and moisture should lead to changes in the relative humidity of the room air. Figure 8 and Figure 7 show the annual courses of temperature and the relative humidity in the test room and in the service room. The results calculated by DELPHIN 5 and DELPHIN 6 are identical. Zone temperatures and relative humidity fluctuate inversely as expected.

As shown in Figure 8, the relative humidity of CHAMPS-BES in the service room began to deviate in the first two days of the year. These deviations caused many convergence errors and slowed down the simulation speed (to a ratio of approximately 1:1 real time / simulation time). Therefore CHAMPS-BES could not finish this variant and the simulation was terminated after 1.25 days of simulation time.

The reason for these deviations was due to an incorrect implementation of the moisture mass balance in CHAMPS-BES. Since the error is limited to air spaces, CHAMPS-BES should be applicable to problems with dominant solids. For this reason, CHAMPS-BES will continue to be tested in the next variant.



Passys-2D-HM-PSBoard/moist\_mass\_integral.out

Figure 5: The total moisture mass of the construction (the sum of all moisture in the construction elements and in the air of both rooms) remains constant throughout the year due to the moisture-proof construction



Figure 6: Annual course of air temperature (T) and relative humidity (RH) of the test room. Zone temperatures and relative humidity fluctuate inversely.



Figure 7: Annual course of air temperature (T) and relative humidity (RH) of the service room. Zone temperatures and relative humidity fluctuate inversely.



Figure 8: First two days of air temperature (T) and relative humidity (RH) of the service room. The results from CHAMPS-BES deviate, which caused convergence errors and CHAMPS-BES could not finish this variant.

# 3 PASSYS-2D-HM-Brick: Moisture buffering in walls with rain load

# 3.1 Differences to the previous variant

In this variant, the moisture behavior of a capillary-active construction is tested. The metal-coated PS foam panels of the partition wall and the east wall are replaced by brick masonry, which implies the use of a moisture-sensitive construction.

# 3.2 Construction

The normal-size PASSYS cell is used as described in section 1.1. All dimensions remain the same. The basic construction (flat roof, floor and west wall) continues to consist of metal-coated PS foam panels. The partition and the east wall are modeled as homogenized brick masonry (Figure 9), i.e. the mortar joints of the masonry are not taken into account. A less water-absorbent material on the surfaces (Brick edge instead of Brick) lowers the water absorption rate.



Figure 9: Discretized normal-size PASSYS cell. The 300 mm metal-coated PS foam panels of the partition and the east wall have been replaced by a moisture-absorbent brick masonry.

# 3.3 Modeling assumptions and parameter settings

The consideration of moisture-absorbing materials should lead to changes in the moisture content in the east wall and have secondary effects on the relative humidity of the room air in the test room. In particular, the following processes are taken into account in addition to the previous variant:

- The moisture boundary conditions (humidity + rain + wind) should have impact on the east wall. Wetting and drying cycles should be observed.
- Depending on the rain load and the material properties, we could see an impact on the room relative humidity and temperature if the external rain water penetrates to the internal surface.

### Appendix 1

The detailed thermophysical properties of the brick are listed in Table 3. For more information such as vapor conductivity function, moisture retention curve, and liquid water transport function please refer to the DELPHIN5 or DELPHIN6 materials database.

	Thermal conductivity in W/mK	Bulk density in kg/m³	Specific heat capacity in J/kgK	Open porosity in m³/m³	Effective saturation in m <sup>3</sup> /m <sup>3</sup>	Water vapor diffusion resistance factor in -	Water absorption coefficient in kg/m <sup>2</sup> s <sup>-1</sup>
Brick	0.55	1400	1000	0.354	0.319	18.8	0.1773
Brick (edge)	0.99	1979	834	0.253	0.241	167.6	0.0507

Table 3: Materia	parameters o	of Brick	and Brick	(edge)
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#### 3.4 **Simulation results**

As shown in Figure 10, there is an accumulation of moisture. The total moisture content in the PASSYS cell increases from 30 kg to 70 kg within one year. The rain load in combination with the capillary suction of the brick masonry obviously has a stronger effect than the drying potential.



Passys-2D-HM-Brick/moist mass integral.out

Figure 10: Total moisture mass of the construction (the sum of all moisture in the construction elements and in the air) increases due to rain load and water absorption in the brick wall.

It should be noted that the moisture accumulation is a seasonal effect that takes place in spring and autumn and correlates with the intensity of the rain load on the east wall. This depends on the given climate data, the rain load on a horizontal surface, the wind speed and the wind direction.

The differences between DELPHIN5 and DELPHIN6 in the accumulated moisture content, which are shown in Figure 10, are attributed to their different wind-driven rain models. DELPHIN5 uses the model according to (Häupl, Fechner, & Stopp, 1995), which estimates the rain flow density on a building with a fixed height and geometry. This model is no longer supported in DELPHIN6 and instead a model according to DIN EN ISO 15927-3 has been implemented.

DELPHIN 6 was the only tool that could completely run the PASSYS-2D-HM-Brick variant. CHAMPS-BES was unable to calculate this case due to convergence problems. It automatically terminated the simulation at the very beginning of the calculation. The calculation of DELPHIN 5 was stopped manually after 152 days had been reached, which took more than two days of calculation time. Therefore only the results of DELPHIN6 will be analyzed afterwards.



Figure 11: East wall accumulates moisture: Relative humidity fields at Jan-11, Apr-11, Jul-20 and Oct-28 (after 10, 100, 200 and 300 days) calculated by DELPHIN6

The development of the relative humidity field at successive times is shown in Figure 11. It can be clearly seen that the moisture accumulation takes place in the east wall. At the end of the year, almost 100 % RH is reached. Porous materials can store much more moisture than air. The east wall is apparently the main factor in the accumulation of moisture in the construction.





Figure 12: Comparison between wall materials PS-Board and Brick by means of room air temperatures and relative humidity in the test room (above) and service room (below), calculated by DELPHIN6.

The thermal resistance of the PS-Board is of course greater than that of the brick wall. In addition, higher moisture levels in the east wall reduce thermal resistance and a higher drying rate causes more evaporative cooling. These effects affect indoor air temperatures. Comparing the results of PASSYS-2D-HM-Brick and PASSYS-2D-HM-PSBoard (see Figure 12), replacing the PS-Board with a brick wall leads to lower test room temperatures in winter and higher test room temperatures in summer. The effects are more pronounced in the test room than in the service room.

Changes in temperature lead to a change in the relative humidity. Since the relative humidity fluctuates inversely to the temperature, positive temperature differences cause negative relative humidity differences, as can be seen in Figure 12 for both the test room and the service room.

# 4 PASSYS-2D-HM-Brick-small: Moisture buffering in walls with rain load

## 4.1 Differences to the previous variant

In order to ensure a reasonable simulation time, a smaller version of PASSYS cell is created.

# 4.2 Construction

This variant uses the small-size PASSYS cell depicted in Figure 13. The dimensions of both rooms were reduced and the thickness of the 300 mm walls was reduced to 200 mm (including the partition wall and the east wall).



Figure 13: Discretized small-size PASSYS cell. The layout remains unchanged; just the dimensions are reduced and the thermal bridges (H-beams) are removed.

### 4.3 Modeling assumptions and parameter settings

Other modeling settings remain unchanged.

### 4.4 Simulation results

Both DELPHIN5 and DELPHIN6 were able to fully calculate this variant (Figure 14). Although the size of the problem was reduced considerably, DELPHIN5 ran quite slowly. As observed in the previous variant, the accumulated moisture levels differ between DELPHIN5 and DELPHIN6, which was attributed to different wind-driven rain models.

All attempts to calculate this variant with CHAMPS-BES failed. The calculation speed has been drastically slowed down due to convergence problems. The simulation was stopped after 13 days of simulation time. The relative humidity of CHAMPS-BES in both rooms obviously differs from the results of DELPHIN5 and DELPHIN6, as shown in Figure 16 and Figure 16.

For example, a large deviation in the relative humidity of CHAMPS-BES is observed after 5 days. To better localize the source of the error, the relative humidity fields of CHAMPS-BES and DELPHIN6 are compared in Figure 17. The comparison shows that the relative humidity in walls agrees well, but the relative humidity distribution in the air deviates significantly.

### Appendix 1

Due to a number of unsolvable problems in this and previous variants, CHAMPS-BES was excluded from further evaluation. Although this appears to be a severe limitation in the use of CHAMPS-BES, it must be stated that CHAMPS-BES reliably solves hygrothermal problems in porous materials if air spaces can be excluded.



Figure 14: Comparison of moisture accumulation in the construction due to rain load and water absorption calculated by DELPHIN5 and DELPHIN6. The accumulated moisture levels differ between DELPHIN5 and DELPHIN6, which is attributed to different wind-driven rain models.



Figure 15: Comparison of air relative humidity in the test room, the results of CHAMPS-BES are very different. Therefore CHAMPS-BES was excluded from further evaluation.



Figure 16: Comparison of air relative humidity in the service room, the results of CHAMPS-BES are very different. Therefore CHAMPS-BES was excluded from further evaluation.



Figure 17: Comparison of relative humidity fields of CHAMPS-BES (left) and DELPHIN6 (right) after 5 and 7.5 days simulation time, the results of CHAMPS-BES differ in the air spaces.

### Appendix 1

#### 5 PASSYS-2D-HM-Brick-small-norain: Moisture buffering in walls

# 5.1 Differences to the previous variant

A difference in moisture absorption between DELPHIN5 and DELPHIN6 was observed in previous variants. This was attributed to the implementation of a new driving rain model in DELPHIN6. In this variant, it is now checked whether both programs deliver the same results if the rain boundary condition no longer applies. The "norain" handling rules out the influence of wind-driven rain.

#### 5.2 Construction

The small-size PASSYS cell is used - see section 4.1.

#### 5.3 Modeling assumptions and parameter settings

Other modeling settings remain unchanged.

## 5.4 Simulation results

The accumulated moisture contents of the two variants PASSYS-2D-HM-Brick-small and PASSYS-2D-HM-Bricksmall-norain are shown together in Figure 18. The two upper curves show the moisture content with the influence of rain, the lower two without the influence of rain. As expected, the deviations without rain are significantly smaller. This supports the argument that DELPHIN5 and DELPHIN6 give the same results as long as rain is not taken into account.

The general uncertainty in rain modeling is due to many unknown factors, e.g. wind flow patterns around buildings, quite large. Therefore, the deviations between DELPHIN5 and DELPHIN6 are in the uncertainty range and are not considered a problem.



Passys-2D-HM-Brick-small-norain/moist\_mass\_integral.out

Figure 18: Comparison of moisture accumulation results from DELPHIN5 and DELPHIN6 with and without rain load.

# 6 PASSYS-2D-HAM-Brick-verysmall-airchange: Air change with rain load

## 6.1 Differences to the previous variant

The air exchange with the external environment is taken into account. The size of the PASSYS cell is further reduced and the rain load is taken into account again.

# 6.2 Construction

The construction is identical to the previous variant, except that the dimensions of the rooms have been reduced.



Figure 19: Discretized verysmall-size PASSYS cell. The dimensions are further reduced.

# 6.3 Modeling assumptions and parameter settings

The hygrothermal balance equations and air change can be simulated together without having to solve an air mass balance. This approach only takes into account the effects of air changes on humidity and temperature in the discretized volume elements.

The air change rates of the test room and the service room are set to 1 h<sup>-1</sup> and remain constant over time. The air change mode requires a direct air exchange with the outside environment without specifying an air flow path. Other modeling settings remain unchanged.

# 6.4 Simulation results

As shown in Figure 20, the differences between DELPHIN5 and DELPHIN6 in terms of the accumulated moisture content are smaller compared to the previous small-size PASSYS cell with rain load. This is primarily due to the lower height of the moisture-absorbing brick wall.

In addition, a secondary effect can be noticed in Figure 20. The convergence of both curves after day 150 is not observed in the previous small-size PASSYS cell with rain load. This effect can be led back to the drying support provided by the air change during summer time. Since we constantly ventilate both rooms with an

ACH = 1  $h^{-1}$ , the effect of higher moisture absorption in DELPHIN6 due to the newly implemented rain model is compensated. This is an interesting result which shows that all effects must be seen in context.

In addition, a secondary effect can be seen in Figure 20. The convergence of both curves after day 150 cannot be observed in the previous small-size PASSYS cell with rain load. This effect can be attributed to the drying provided by the air change in summer. Since we ventilate both rooms with constantly ACH =  $1 h^{-1}$ , the effect of higher moisture absorption in DELPHIN6 (due to the new rain model) is compensated. This is an interesting result, which shows that all effects have to be seen in context.

The next question is how the relative humidity in the indoor air is affected by this scenario. Therefore, the comparison of DELPHIN5 and DELPHIN6 focused on the greatest difference between days 140 and 150. As shown in Figure 22, the different moisture absorption in the walls has hardly any influence on the relative humidity in the rooms. This can be explained by the dominant air change rate in this variant.







Figure 21: Comparison of relative humidity in the service room between days 140 and 150



Figure 22: Comparison of relative humidity in the test room between days 140 and 150

# 7 PASSYS-2D-HAM-Brick-verysmall-airchange-norain: Air change

# 7.1 Differences to the previous variant

Similar to the previous variants without air change, this variant checks whether both programs deliver the same results if the rain boundary condition no longer applies. The "norain" handling rules out the influence of wind-driven rain.

# 7.2 Construction

The verysmall-size PASSYS cell is used - see section 6.1.

# 7.3 Modeling assumptions and parameter settings

Other modeling settings remain unchanged.

## 7.4 Simulation results

The accumulated moisture contents of the two variants PASSYS-2D-HM-Brick-verysmall-airchange and PASSYS-2D-HM-Brick-verysmall-airchange-norain are shown together in Figure 23. The two upper curves show the moisture contents with rain, the lower ones without. It was expected that the deviations should become smaller without rain, which is not the case.

The deviations between DELPHIN5 and DELPHIN6 for the cases without rain begin on day 150 and accumulate until day 300. This is exactly the period in which the air change drying has the dominant effect, which is concluded from the convergence of the upper curves during this period. This problem is still unsolved and should be investigated further. The issue should be taken into account for future updates of the DELPHIN software.



Figure 23: Comparison of moisture accumulation results from DELPHIN5 and DELPHIN6 with and without rain load.



Figure 24: Comparison of relative humidity in the service room and the test room, both calculated by DELPHIN6

# 8 PASSYS-2D-HAM-Brick-verysmall-airgap-norain: Air flows

# 8.1 Differences to the previous variant

In the previous "airchange" variants, direct air exchange with the outside environment without specifying an air flow path was assumed. Now the air flow path is determined and a pressure-driven air flow is generated through the entire PASSYS cell.

# 8.2 Construction

The verysmall-size PASSYS cell is used - see section 6.1. The construction is made air permeable by inserting air gaps at the connections between vertical and horizontal components. Figure 25 shows the upper airflow path, which consists of three wall-roof connections. The upper and lower air flow paths are connected to the indoor air volume of both rooms, creating a continuous air flow through the entire PASSYS cell.



Figure 25: Discretized verysmall-size PASSYS cell with specified air flow path.

# 8.3 Modeling assumptions and parameter settings

In contrast to the "air exchange" mode, the "air gap" mode requires the solution of an air mass balance equation. The corresponding primary solution variable is the volumetric density of the air in each discretized volume element. Secondary state variables, e.g. the gas phase (or air) pressure is calculated using the DELPHIN decomposition algorithm. The air pressure field and its gradients as well as the air mass flows and their divergences are continuously calculated in each iteration step.

The time constants for pressure equalization in the gas phase are very small compared to those for temperature or humidity equalization. Therefore, DELPHIN5 and DELPHIN6 solve the air mass balance equation in a quasi-stationary mode, i.e. the pressures are kept constant over a time step and updated at the beginning of the next time step. Typical time steps for pressure equalization are in the range of one minute.

Solving an air mass balance equation requires boundary and initial conditions. The air inlet pressure on the east side is 101327 Pa, the air outlet pressure on the west side is 101325 Pa. This creates an overpressure of 2 Pa at the inlets and a directed air flow through the construction from east to west. Note that the volumetric flow (m3/h) is constant per se, while the respective air change rates (volumetric flow divided by air volume) differ between the test room and the service room (see Figure 25). The pressure difference leads to higher air change rates (2.6 and 2.5 h<sup>-1</sup>) than the specified value of 1 h<sup>-1</sup> in the previous variant. The initial pressure field is calculated at the beginning of the simulation by pressure equalization under the given boundary conditions.

Finally, it should be noted that the solution to the air mass balance equation is not a CFD simulation. A CFD simulation is based on the solution of the momentum balance equation, which is much more demanding in terms of physics and computing load. CFD should also deliver a higher level of accuracy. Solving an air mass balance could be sufficient for problems with a clearly dominant pressure-driven flow. The focus of such problems is on the effects of airflow on temperature and humidity distribution. A solution to the air mass balance only may be too imprecise for problems dominated by buoyancy.

### 8.4 Simulation results

This variant leads to higher air change rates, which can be seen in Figure 26 from the two lowest pairs of curves without rain. The moisture accumulation over the course of the year is lower than in the previous variant with a given air change rate. The difference in moisture content between DELPHIN 5 and DELPHIN 6 also becomes smaller. The unresolved problem with air change drying obviously has to do with the construction's ability to release moisture into the indoor air under air change conditions.

In the "airgap" mode, the service room receives "preconditioned" air from the test room with a certain time delay, which depends on the air flow rate. The relative humidity in the service room and in the test room are shown in Figure 27. The comparison with Figure 24, which shows the "airchange" case, is interesting. The amplitudes of the relative humidity in the service room are smaller and shifted in time while the curves in the "airchange" case run almost parallel. The time difference is likely to depend on the distribution of moisture in the air of the test room. There is no well-mixed assumption that is normally used by whole building simulation programs that model the indoor air with just one node. The air volume is discretized in DELPHIN5 and DELPHIN6, which leads to a certain duration of a moisture wave through the entire PASSYS cell.

As indicated in Figure 25, the air velocity in the air gaps was given as 3 cm/s. The expected air mass flow density can be calculated at 36 g/m<sup>2</sup>s (see formula below). In Figure 29, however, airflow fluctuations can be seen at both the inlet and outlet points, which occur mainly in the time of moisture accumulation. DELPHIN5 and DELPHIN6 show this behavior in the same way.

$$j_g = \rho_g \cdot v_g = 1200 \frac{\text{g}}{m^3} \cdot 0.03 \frac{m}{s} = 36 \frac{g}{m^2 s}$$
 Air mass flux density in g/m<sup>2</sup>s

One explanation for these fluctuations could be that the air gaps are sometimes clogged due to moisture condensation. A moisture dependency is implemented in the DELPHIN code that linearly reduces the convective air flow with increasing moisture content. The convective airflow is completely blocked when the material saturated. From this hypothesis it can be concluded that the lower inlet and the lower outlet can

### Appendix 1

sometimes become saturated with water due to condensation processes. The reduced mass flow densities are indicated by the zero peak values of the black curves in Figure 28 and Figure 29.

Blocking the lower air flow paths forces the upper ones to increase their air velocities. This would explain the higher mass flow rates at the top inlet and outlet. This hypothesis has to be checked by carefully monitoring the processes in the air gaps, which was not part of this exercise.



Passys-2D-HAM-Brick-verysmall-airchange-norain/moist\_mass\_integral.out

Figure 26: Comparison of moisture accumulation results from DELPHIN5 and DELPHIN6 with and without rain load and under different air change conditions.



Figure 27: Comparison of relative humidity in the service room and the test room, both calculated by DELPHIN6



#### Figure 28: Air mass flow density at inlet positions





# **References**

Häupl, P., Fechner, H., & Stopp, H. (1995). *A Study of Driving Rain.* Paper presented at the Feuchtigkeit im Mauerwerk. Feuchtetag '95 - Messen, Berechnen, Trockenlegen., Berlin.

# **Appendix 2: 3D Simulation results**

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# 1 Base case – Test case T100

### Short description: Base case with only heat conduction



Graph: Air Temperature – Test Room [°C]

Analysis:





- All programs are located in a small range CV(RMSE) < 10%
- Biggest deviation from Energy Plus CV(RMSE) =3.5%

# 2 Construction test cases

### 2.1 Test case T201 – Heavy Construction

### Short description: South wall replaced with a heavy construction

### Graph: Air Temperature – Test Room [°C]



Analysis:





NANDRAD	EnergyPlus	IDA ICE	TRNSYS	Modelica	DYNBIL
ref	++	++	++	++	++

- All programs are located in a small range CV(RMSE) < 10%
- Biggest deviation from IDA ICE CV(RMSE) ≈3.8%

### 2.2 Test case T202 – Ground Contact

#### Short description: Base case with ground contact on the floor



### Graph: Air Temperature – Test Room [°C]

Analysis:





- All programs are located in a small range CV(RMSE) < 10%
- Except IDA ICE has large deviation CV(RMSE) ≈35.8%
- IDA ICE has a higher heat flux over the floor construction
- Seems to be a different ground model

### 2.3 Test case T203 - Window (only Heat Transmission)

Short description: Base case with a window in the south wall and only heat transmission



Graph: Air Temperature – Test Room [°C]

Analysis:



- All programs are located in a small range CV(RMSE) < 10%
- Except IDA ICE has a slightly larger deviation CV(RMSE) ≈ 7.8%
- IDA ICE Air Temperature reacts more slowly

# 3 Outdoor Climate test cases

## 3.1 Test case T301 – Short Wave Radiation

### Short description: Base case with short wave radiation on the outside surfaces



Graph: Air Temperature – Test Room [°C]

### Analysis:





- All programs are located in a small range CV(RMSE) < 10%
- Due to slightly different sun position models and therefore different solar radiation loads the deviation between the programs increases slightly
- TRNSYS Air Temperature is lower during summer
- IDA ICE Air Temperature is higher during winter

# 3.2 Test case T302 – Long Wave Radiation

Short description: Base case with long wave radiation on the outside surfaces



Graph: Air Temperature – Test Room [°C]

Analysis:



# Analysis - T302 Long Wave Radiation (outside)

- NANDRAD, EnergyPlus, Modelica and DYNBIL are located in a small range CV(RMSE) < 10%
- Except TRNSYS has a larger deviation CV(RMSE) ≈ 25.2 %
- TRNSYS seems to have a different model for long wave radiation

### 3.3 Test case T303 - Convection Coefficient

Short description: Base case with dynamic convection coefficients on the outside surfaces



Graph: Air Temperature – Test Room [°C]

Analysis:



#### Analysis - T303 ConvectionCoefficient

- NANDRAD has no model for dynamic convection coefficients
- EnergyPlus has been set as reference since all programs are close
- All programs are located in a small range CV(RMSE) < 10%
- IDA ICE has the largest deviation CV(RMSE) ≈ 7.8 %
- IDA ICE Air Temperature reacts more slowly

## 3.4 Test case T304 – Combination of T301, T302, T303

Short description: Combination of test cases T301, T302 and T303



Graph: Air Temperature – Test Room [°C]

Analysis:



Analysis - T304 Convection Coefficients

- Energy Plus has been set as reference
- NANDRAD has no model for dynamic convection coefficients
- All programs are located in a small range CV(RMSE) ≤ 10%
- Except IDA ICE has a larger deviation CV(RMSE) > 30%
- IDA ICE Air Temperature is overall lower than the other programs
#### Appendix 2

#### 4 **Indoor Climate test cases**

## 4.1 Test case T401 – Long-Wave Radiation

Short description: long-wave emission coefficient of all inside surfaces set to 0.87.





#### Analysis:



#### Analysis - T401 Long Wave Radiation (inside)

NANDRAD	EnergyPlus	IDA ICE	TRNSYS	Modelica	DYNBIL
ref	++	+	++	++	++

- IDA ICE Air Temperature reacts more slowly \_
- All programs are located in a small range  $CV(RMSE) \le 10\%$
- IDA ICE has the largest deviation  $CV(RMSE) \approx 6.8\%$ \_

# 4.2 Test case T403a - Simple Window Model without angle dependence

**Short description:** Simple Window Model without angle dependent SHGC-factor in the south wall of the passys cell



Graph: Air Temperature – Test Room [°C]

#### Analysis:



#### Analysis - T403a Simple Window Model without angle dependence

- Large gap between all programs
- Energy Plus has no angle independent SHGC-factor
- Seems like the angle independent SHGC-factor is considered differently in each program
- Only DYNBIL and NANDRAD are close to each other CV(RMSE) < 10%

#### **4.3** Test case T403b - Simple Window Model with angle dependence

Short description: Simple Window Model with angle dependency in south wall



Graph: Air Temperature – Test Room [°C]

#### Analysis:





- TRNSYS and NANDRAD are close to each other  $CV(RMSE) \le 10\%$ \_
- Modelica and NANDRAD are slightly off but still close to each other CV(RMSE) ≈ 10%

#### Test case T404 - Combination of T401 and T403b (if not available T403) 4.4

Short description: Combination of T401 and T403b (if not available T403)



Graph: Air Temperature – Test Room [°C]

#### Analysis:





- NANDRAD, TRNSYS and Modelica are located in a small range CV(RMSE) ≤ 10%
- DYNBIL is off and constantly has a lower Air Temperature especially during summer \_

#### 4.5 Test case T405a - Detailed Window Model with angle dependence

Short description: Detailed Window Model with angle dependency in south wall



Graph: Air Temperature – Test Room [°C]

Analysis:





- IDA ICE reference due to high air temperatures in NANDRAD -
- NANDRAD has no angle dependent SHGC-factor in detailed window mode at the moment
- IDA ICE lies in between all air temperature curves
- In general big gap between all programs \_
- Only IDA ICE, Modelica and EnergyPlus lie close together– CV(RMSE) ≤ 11% \_

# 4.6 Test case T405b - Detailed Window Model: angle dependency & internal radiation distribution

**Short description:** Base Case with detailed Window Model with angle dependency in south wall and internal radiation distribution





Analysis:





- NANDRAD and DYNBIL are close to each other  $CV(RMSE) \le 10\%$
- TRNSYS is far off compared to NANDRAD and DYNBIL
- TRNSYS seems to have an input error or a different detailed window model which leads to significant differences regarding the Air Temperature of the test room

# **5** Internal Loads test cases

# 5.1 Test case T501 - Internal Heat Loads

#### Short description: Base case with internal convective heating loads

# Graph: Air Temperature – Test Room [°C]



Analysis:



- All programs are located in a small range CV(RMSE) ≤ 10%
- IDA ICE has the largest deviation CV(RMSE) ≈ 6%

# 5.2 Test case T502 - Internal Heat Loads with convective/radiative split

Short description: Base case with internal convective and radiative heat loads



Graph: Air Temperature – Test Room [°C]

#### Analysis:



- All programs are located in a small range CV(RMSE) ≤ 10%
- IDA ICE has the largest deviation CV(RMSE) ≈ 8%

# 6 Infiltration test cases

## 6.1 Test case T601 - Constant Infiltration

#### Short description: Base case with constant infiltration

### Graph: Air Temperature – Test Room [°C]



Analysis:





- All programs are located in a small range CV(RMSE) ≤ 10%
- IDA ICE has the largest deviation CV(RMSE) ≈ 6%

# 6.2 Test case T602a - Infiltration defined by design flow rate – temperature driven

Short description: Base case with infiltration defined by temperature driven design flow rate



Graph: Air Temperature – Test Room [°C]

#### Analysis:





- TRNSYS set as reference
- NANDRAD only has a simple infiltration model
- All programs are located in a small range CV(RMSE) ≤ 10%
- Modelica has the largest deviation CV(RMSE) ≈ 6%

#### Test case T602b - Infiltration defined by design flow rate - wind driven 6.3

Short description: Base case with infiltration defined by wind driven design flow rate



Graph: Air Temperature – Test Room [°C]

Analysis:



Analysis - T602b Infiltration defined by design flow rate - wind driven

- TRNSYS set as reference \_
- NANDRAD only has a simple infiltration model
- All programs are located in a small range CV(RMSE) ≤ 10%
- Modelica has the largest deviation CV(RMSE) ≈ 4.2% \_

# 6.4 Test case T602 - Infiltration defined by design flow rate – wind & temperature driven

Short description: Base case with infiltration defined by wind and temperature driven design flow rate



Graph: Air Temperature – Test Room [°C]

#### Analysis:

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- TRNSYS set as reference
- NANDRAD only has a simple infiltration model
- All programs lie in a small range CV(RMSE) ≤ 10%
- Modelica has the largest deviation CV(RMSE) ≈ 5.9%

# 6.5 Test case T603 - Wind speed and stack effect dependent infiltration

Short description: Base case with wind speed and stack effect dependent infiltration



Graph: Air Temperature – Test Room [°C]

#### Analysis:



- TRNSYS set as reference
- NANDRAD only has a simple infiltration model
- All programs are located in a small range CV(RMSE) ≤ 10%
- IDA ICE has the largest deviation CV(RMSE) ≈ 6.8%

# 6.6 Test case T604 - Overflow Case

Short description: Base case with overflow case (inaccurate test case description)



Graph: Heating Rate – Test Room [°C]

Analysis:





- TRNSYS set as reference
- No air flow between zones shown since variation is too big only heating rate is shown
- Problems in the test case due to redundant information in text and graphic of the test case document,
  IDA ICE uses V=20 m<sup>3</sup>/h and all other tools 30 m<sup>3</sup>/h
- NANDRAD only has a simple infiltration model
- Test case needs to be adjusted/specified

# 6.7 Test case T605 - Realistic Case: Combination of T603 and T604

**Short description:** Combination of the test case T603 and T604 Wind speed and stack effect dependent infiltration combined with an overflow Case (inaccurate test case description)



Graph: Air Temperature – Test Room [°C]

#### Analysis:





- TRNSYS set as reference
- No air flow between zones shown since variation is too big only Air Temperature is shown
- NANDRAD only has a simple infiltration model
- Different room temperatures due to different overflow rates
- Test case needs to be adjusted/specified

# 7 Heating/Cooling test cases

# 7.1 Test case T701a Constant Ideal Heating

#### Short description: Base case with Constant Ideal Heating to 21°C

- **Graph 1:** Air Temperature Test Room [°C]
- Graph 2: Heating Rate Test Room [W]



#### Analysis:



- All programs are located in a small range considering the Air Temperature CV(RMSE) ≤ 10%
- Except Modelica has a more significant deviation of up to 1K difference to the heating setpoint CV(RMSE) ≈ 2.8%
- IDA ICE has a decreased annual heating load (-15% deviation)

# Appendix 2

# 7.2 Test case T701b Constant Ideal Cooling

Short description: Base case with Constant Ideal Cooling to 3°C

**Graph 1:** Air Temperature – Test Room [°C]

Graph 2: Cooling Rate – Test Room [W]



#### Analysis:



Analysis - T701b Constant Ideal Cooling

- All programs are located in a small range considering the Air Temperature  $CV(RMSE) \le 10\%$
- Except Modelica has a more significant deviation of up to 1K difference to the heating setpoint CV(RMSE) ≈ 3%
- IDA ICE has a decreased cooling load (-16% deviation)

# 7.3 Test case T701 Ideal Heating/Cooling

Short description: Base case with Constant Ideal Heating/Cooling controlled by schedule

```
Graph 1: Air Temperature – Test Room [°C]
```

Graph 2: Heating Rate – Test Room [W] Graph 3: Cooling Rate – Test Room [W]



## Analysis:





Annual Heating-/CoolingLoad Constant Ideal Heating/Cooling [kWh/a]





	NANDRAD	EnergyPlus	IDA ICE	TRNSYS	DYNBIL	Modelica
Air	ref	++	++	++	++	-
Heating	ref	++	-	++	++	-
Cooling	ref	++	-	++	++	+

- Modelica is strongly oscillating around the setpoint temperatures and has therefore large deviations to the other programs
- Modelica also seems to be shifted due to probably wrong weather data
- IDA ICE has also increased deviations in annual heating and cooling energy demand since the heating and cooling rate is constantly lower than the other programs

# 7.4 Test case T702 Surface Heating/Cooling

Short description: Base case with Constant Ideal Heating/Cooling controlled by schedule and done only by radiation

- **Graph 1:** Air Temperature Test Room [°C]
- Graph 2: Heating Rate Test Room [W]
- Graph 3: Cooling Rate Test Room [W]



T702 – Surface Heating/Cooling - Air Temperature

## Analysis:



- TRNSYS set as reference
- Modelica is strongly oscillating
- Heating and Cooling Rate are permanently too high
- Both programs are barely comparable
- Testing surface cooling is not always suitable for each program.
- Test case needs to be adjusted/specified

# 8 Hygrothermal test cases

# 8.1 Test case T801 Include moisture balance without moisture source

**Short description:** Test case based on T604 but with hygrothermal calculation and no moisture-buffering in walls (inaccurate test case description)





Analysis:





- TRNSYS set as reference
- Errors in input data in all programs due to inaccurate test case
- IDA ICE and DYNBIL heat room air to constant 20°C; TRNSYS and Modelica do not heat the air
- Results are barely comparable; Test case needs to be adjusted/specified

# 8.2 Test case T802 Include moisture balance with moisture source (schedule)

**Short description:** Test case based on T604 but with hygrothermal calculation and with moisture-buffering in walls (inaccurate test case description)





Analysis:



- TRNSYS set as reference
- Errors in input data of all programs due to inaccurate test case
- IDA ICE and DYNBIL heats room air to constant 20°C
- TRNSYS and Modelica do not heat the air
- Modelica has also large deviations and there seems to be an error in the input data for the simulation
- Test case needs to be adjusted/specified

# 8.3 Test case T803 Include moisture balance with moisture source and buffer effects

**Short description:** Test case based on T604 but with hygro-thermal calculation, with moisture-buffering in walls and a moisture source in the test room (inaccurate test case description)



Graph: Absolute Humidity – Test Room [g/kg]

#### Analysis:





- TRNSYS set as reference
- Errors in input data in all programs
- Test case needs to be adjusted/specified
- IDA ICE and DYNBIL heats room air to constant 20°C
- TRNSYS and Modelica do not heat the air

#### Appendix 2

# 9 Pollutants test cases

# 9.1 Test case T901 Include inert pollutant (CO2)

**Short description:** Test case based on T604/T802 but with a scheduled CO2 source in the test room (inaccurate test case description)

Graph: CO2 Concentration – Test Room [g/kg]



### Analysis:



Analysis - T901 CO2

- TRNSYS set as reference
- Results are barely comparable
- Test case needs to be adjusted
- Simple Infiltration model should be used for this test case
- Test case needs to be adjusted/specified

# 9.2 Test case T902 Combine inert pollutant (CO2) with natural ventilation

**Short description:** Test case based on T605 combined with test case T901 – means a scheduled CO2 source in the test room



Graph: CO2 Concentration – Test Room [g/kg]

#### Analysis:





- Errors in input data due to faulty test case T604 description
- Results are barely comparable