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Opportunities and pitfalls of using building performance simulation in explorative R&D contexts

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One of the promising use cases of building performance simulation (BPS) is its role as a virtual laboratory in research and development (R&D) projects that aim to bring innovative building components from initial idea towards market introduction. By facilitating what-if explorations and whole-building insights, BPS can create complementary value, alongside actual experiments. However, explorative R&D projects tend to be rather erratic and are more ill-defined than typical BPS tasks. This raises several issues concerning application, interpretation and communication of BPS-based performance predictions in explorative contexts. The aim of this paper is to highlight opportunities and potential pitfalls of the use of BPS in this application domain. First, the characteristic properties of exploration-driven R&D projects are contrasted with more conventional BPS projects using a systematic requirements engineering approach. Then, the process and outcomes of three R&D projects of innovative façade systems are discussed. Finally, the lessons learned from these studies are presented.

Keywords: modelling and simulation; virtual experiments; product development; adaptive facades

1. Introduction

Over the last decades, building performance simulation (BPS) has evolved to become an established tool for supporting the design and operation of high-performance buildings (Clarke and Hensen 2015). BPS can facilitate analysis of the interrelated effects of building shape, construction type, materials, energy systems, weather influences and occupant behaviour on building performance. The potential of BPS is most pronounced when it is proactively used for guiding building design decisions towards solutions that combine high indoor environmental quality (thermal, air quality, visual, acoustic) with minimum use of resources (e.g. CO_2 emissions or materials) (Clevenger and Haymaker 2011). The tool is sometimes said to act as a virtual laboratory, capable of servicing computational experiments that can test different what-if scenarios, perform design space explorations and provide insights into the propagation of uncertainties (Augenbroe 2011). However, the traditional, and still most common use of BPS is the application by engineers, for 'post-rationalization' and code compliance at a time in the building design process when many influential design decisions have already been made (Attia et al. 2012; Bernal, Haymaker, and Eastman 2015). The product and process-related enhancements that are necessary to thoroughly and routinely encapsulate BPS in active design processes remain, therefore, work in progress (Clarke 2015).

In an abstract way, the majority of building design processes can be described as the activity of conjoining various spatial configurations with different combinations of existing components, technologies and building material assemblies until a solution is found that satisfies all aesthetic and functional requirements (de Wilde and Van der Voorden 2004). This is also the setting in which BPS usually operates. The pattern of selecting from a set of known or proven solutions is quite rigid, and often gives little room for conceiving truly innovative building concepts that reconsider the way in which buildings operate. It is increasingly realized, however, that such breakthrough innovations are necessary to meet the twenty-first century's societal and environmental challenges for a sustainable built environment (IEA 2013). Building envelopes can play a crucial role in this respect, and in particular, the concept of adaptive facades has regularly been identified as being among the most promising development trends (COST 1403 2015; Loonen et al. 2013).

Before new building products and components become available on the market, there is typically a preceding process of iterative product development cycles in which multiple technology readiness levels are sequentially addressed (Larsson, Sundqvist, and Emmitt 2006). During these developments, special attention should be paid to transforming the innovations into scalable building envelope

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elements and products, to be able to achieve the biggest overall impact (Sariola 2018; Winch 1998).

New ideas for innovative building envelope systems and materials can originate from many different directions (Loonen 2018). On the one hand, they can derive from creativity-driven endeavours such as projects in architecture schools, collegiate competitions (Cronemberger et al. 2014) and design contests (Lampel, Jha, and Bhalla 2012). On the other hand, new ideas can also emerge from research projects with more fundamental science orientation (Bastiaansen et al. 2013; Lee et al. 2013) or by seeking cross-overs with neighbouring fields of science and technology such as biology (Badarnah and Kadri 2015; Loonen 2015) or robotics (Rossi, Nagy, and Schlueter 2012).

A common factor in the R&D processes described above is the need for experimentation, either conceptually or physically, in the form of prototypes (Thomke 1998). Sometimes this happens in a qualitative way, but generally, there is also a need for quantitative expressions of performance, for the validation of ideas and as a measure of how the proposed problem-solution pair compares to common practice or alternative developments (Bernal, Haymaker, and Eastman 2015; O'Connor and Veryzer 2001). Such comparisons can either happen on the component or on the whole-building level, in which the latter case tends to provide the richest feedback to the development team (Loonen et al. 2014). Owing to the characteristics that make BPS suitable for providing informed decision-making in building design processes, it is argued that the same tools and methods can also be used in a virtual laboratory setting to provide quantitative guidance in R&D projects. However, based on a previous review of building product development processes (Loonen et al. 2014), and inferring from the paucity of BPS-supported applications obtained through a literature search in the leading journals 'Construction and Building Materials', 'Advanced Energy Materials', 'Nature Materials' and 'Energy & Environmental Science', it turns out that, despite its potential, BPS is rarely used for supporting such exploratory developments.

It is likely that the restricted use of BPS in R&D and product development is due to the fact that the explorative, iterative and diverging features of such projects do not always match with the analysis- and evaluation-oriented attributes of BPS. Despite this apparent mismatch, the premise of this article is that, provided that it is used in a sensible and sometimes creative way, there is much scope for BPS as a support tool for decision-making throughout various phases of ill-defined, design-oriented R&D projects of innovative responsive façade concepts. The goal of this paper is to examine opportunities and pitfalls of using BPS in explorative R&D contexts. Once such considerations are better understood, it can potentially open up a new application domain and corresponding user base for wider deployment of the advantageous aspects of BPS.

The remainder of this paper is split into two main parts. The first part (Section 2) will analyze the requirements and challenges for performance prediction in R&D projects from a problem formulation perspective. In the second part, the process of introducing simulation-assisted decision-making in three multi-disciplinary R&D projects will be described for illustration purposes (Section 3), covering: (i) a hollow-core façade slab, ventilated with outside air to make effective use of thermal mass, (ii) a 3d-printed façade component with water-carrying channels for nocturnal heating and cooling, and (iii) a switchable glazing system with controllable reflection in the near-infrared part of the spectrum. Results from a series of simulation studies (e.g. materials selection, design of laboratory experiments, comfort prediction and risk quantification) that focus on different temporal and spatial scales are presented, followed a by a critical reflection on their application and the lessons learned. The paper concludes by generalizing the observations from the case studies into an overview of strengths and challenges for more widespread use of BPS to support future innovation processes.

2. Requirements and challenges from a problem formulation perspective

Guidelines for successful modelling and simulation studies subdivide the simulation life-cycle into a number of steps (Balci 1990; Zeigler, Kim, and Praehofer 2000). The first step of 'problem formulation' is arguably the most important one, because it provides the foundation for ensuring that the outcomes of a simulation study match with the expectations of relevant stakeholders (Robinson and Pidd 1998). It turns out, however, that in most practical cases, the problem formulation step is rarely addressed in a formal way (Pidd 2007). Based on an extensive literature review, six requirements for structured problem formulation were identified by Balci and Nance (1985):

(1) Establish the problem domain boundary.
(2) Gather data and information about the problem domain within the established boundary.
(3) Identify the stakeholders and decision makers who would be interested in the solution of the communicated problem.
(4) Specify the needs and objectives of the stakeholders and decision makers identified.
(5) Identify and specify the constraints.
(6) Specify all assumptions made clearly and explicitly.

The type of projects that we address in this paper share many similarities with the class of ill-defined (Lynch et al. 2009) or ill-structured problems (Simon 1973). Such projects typically (i) have vaguely stated goals; (ii) are open-ended and do not lead to unambiguously right or wrong answers; (iii) involve unstated or assumed problem constraints; and (iv) require a large database of relevant information that is often difficult to access.

The ill-defined nature of design-oriented building envelope R&D projects is hardly compatible with the six problem formulation requirements presented above. To be able to use modelling and simulation in a meaningful way, there is therefore often a need for *recharacterization* of the problem. This process may include redefining aspects of the problem to relate it to relevant domain rules and concepts; identifying clear solution criteria; reinterpreting essential rules and concepts according to the present goal; and analogizing or distinguishing the current problem from prior cases (Goel and Pirolli 1992; Lynch et al. 2009).

Albeit challenging, appropriate formulation and recharacterization of the problem at hand can significantly enhance the opportunities for valuable use of BPS in R&D projects, compared to the regular ad hoc approaches. There are nevertheless a number of challenges that can hinder integration of simulation support in the process:

- There is often a mismatch between (i) the amount and level-of-detail of available information about the concept under development (e.g. drawings, thermophysical properties, control strategies), and (ii) what is needed as input for BPS programs. The model abstraction process needs to be done carefully, finding a balance that reconciles inputs for uncertain and undecided design parameters with the confidence range that is needed to address the question (Rezaee et al. 2015).
- The modelling capabilities of BPS software tools have the tendency to lag behind the market availability of innovative façade components (Loonen et al. 2017). Many simulation tools do therefore not have the component models or algorithms required to predict the performance of certain novel building systems and materials. The use of workaround approaches may be required.
- The output options of simulation programmes can be perceived as not informative for timely assistance in the decision-making process. An example is the use of annual performance metrics, which are often required by compliance-driven simulation tasks, when information at higher temporal granularity can sometimes be more suitable to quantify the performance of innovative technologies. Similar issues have been observed in interdisciplinary building design processes (Bleil de Souza 2012).
- The time required to obtain accurate predictions can be incompatible with the need for quick feedback.
- It is not uncommon that problems and proposed solutions are co-evolving during the project. Intermediate solutions often expose hidden aspects and can trigger the redefinition of the problem (Bernal, Haymaker, and Eastman 2015; Dorst and Cross 2001). This implies that simulation strategies must continuously be adapted to new conditions, favouring the use of agile modelling approaches.
- Team members in R&D projects tend to have a very diverse professional background. Their ways of working and approach to problem solving can be markedly different (Alsaadani and Bleil de Souza 2016). This highly multi-disciplinary character leads to a significant need for expectation management, especially when collaborators from different scientific fields are involved. Not all team members are familiar with the capabilities and limitations of BPS tools, and moreover, they are unaware of underlying assumptions, or how results should be interpreted.
- Contrary to regular building design tasks, there is usually no defined object to which the new technology should be applied. This translates into a need to develop reference building models that are either characteristic for a larger part of the building stock, or that represent a specific building type. It may not be straightforward to find a right balance between generalizability and still representing the typical irregularities that any building has.
- In addition to the previous point, there is usually no clear idea about the application area (i.e. location) in which the technology has the highest potential (Hensen et al. 2015). Climate scoping studies such as the work by DeForest et al. (2013), Causone (2016), Belleri et al. (2018), and Juaristi et al. (2018) can be carried out, but there is little guidance about how such studies are best performed.

3. Case studies

By discussing the process and outcomes of three innovation projects, this paper illustrates some characteristic challenges and opportunities of proactive integration of BPS in exploratory R&D projects. All three selected projects were part of the so-called *4TU-Bouw Lighthouse* programme, a joint funding scheme established by the Architecture and Civil Engineering departments of the four universities of technology in the Netherlands. *4TU-Bouw Lighthouse* projects are quite different from most other research project calls, as the evaluation criteria of the proposals specifically address the 'imaginative' nature of the research, as well as the delivery of tangible results (e.g. prototypes or test environments) with a focus on technological advancement in the which economic competitiveness of the final solution is initially of lower importance. The relatively short project duration of one year and the need for collaboration between universities and across disciplines appeals to 'fast-track' and 'high-risk' proposals that will ultimately lead to a proof of concept or proof of failure. Although the three projects were carried out in a multi-disciplinary setting in which different team members fulfilled different complementary roles, this paper primarily focuses on the building physics and energy efficiency subdomains.
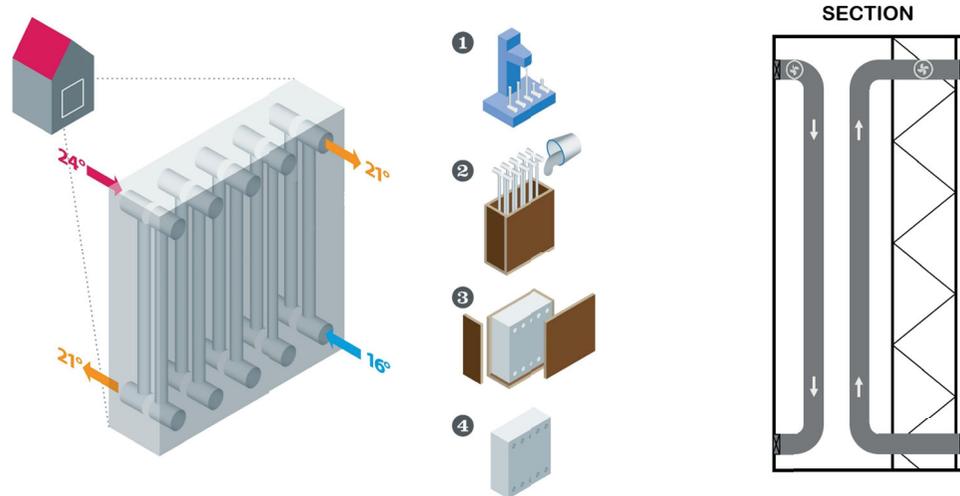
Figure 1.   Convective concrete concept.

3.1.   Case study 1 – convective concrete

3.1.1.   System description

The main goal of Convective Concrete is to mitigate residential overheating during summer periods by reducing the temperature of constructions during building operation through active heat exchange between the building construction and cool outside air at night (de Witte, Knaack, et al. 2017). To accomplish the on-demand charging of thermal mass, a network of ducts is embedded in an externally insulated concrete wall element. This design is accomplished by developing customized formwork elements in combination with advanced concrete mixtures.

Using Fused Deposition Modeling (FDM), an Additive Manufacturing (AM) process based on material extrusion, the air channels are printed in wax so they can be placed in the formwork before casting the concrete and then be melted after the concrete is hardened (Figure 1). Consequently, the concrete is in direct contact with the convective airflow that circulates through it, and each air channel can be unique in form to optimize the performance of the system. The convection takes place with separate pipes on both sides of the concrete's core to increase the charge/discharge of the thermal storage process. The airflow rate through the wall elements is controlled with the help of dampers and small computer fans with a power consumption of 0.5 W each.

3.1.2.   Simulation at the element scale

Although the design process made extensive use of experimentation through the making of mock-ups, not all parameters and design options could be tested this way, due to time and material constraints. The purpose of using computational simulations was to assist decision-making for a number of selected variables in order to select the most promising properties to further analyze with the mock-up. It is noted that the heat transfer phenomena in Convective Concrete have a three-dimensional character. However, given (i) the type of questions that were to be addressed at this early technology readiness level, (ii) the time available to ensure that the outcomes of the simulations could actively inform the development direction of the mock-up, and (iii) the large number of undecided parameters in terms of thermophysical properties and geometric design, it was decided that a two-dimensional model would be most fit-for-purpose. The software program Energy2D was used to solve the dynamic Fourier heat transfer equations for the Convective Concrete case, to aid in making decisions on the shape and layout of the air channels in the Convective Concrete panel as well as the properties of the concrete mixture itself. Energy2D is a relatively new programme (Xie 2012) and is not yet widely used as a building performance simulation tool. To gain more confidence in the predictions with Energy2D, an analytical validation study was first carried out, inspired by the approach described by Hensen and Nakhi (1994). This validation study showed that the simulation results never divert more than 0.45°C (de Witte, De Klijn-Chevalerias, et al. 2017) from the exact solution and it was therefore considered acceptable to further use this model.

Energy2D was then used to calculate and visualize the dynamic heat dissipation for various layouts of air channels. Different shapes, sizes and distributions of air channels were tested in a plan view and the isotherms were observed to determine the most efficient configuration. Figure 2 presents the comparison of aligned and staggered air channel distributions paused at the same time during the simulation.

From this study, the first mock-up was designed with round air channels with a diameter of 4 cm which are aligned with a spacing of 8 cm between them.
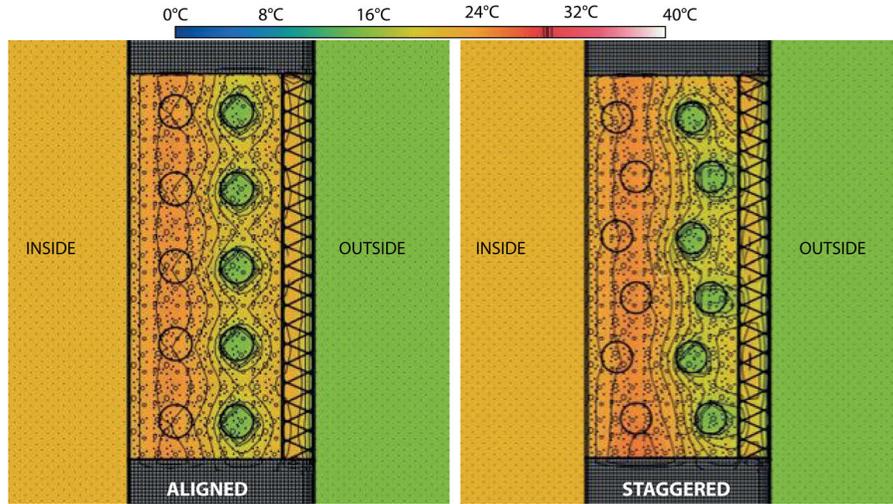
Figure 2. Staggered and aligned distribution of air channels.

Convective Concrete relies on thermal energy storage as an enabler for night-time release of the casual and solar heat gains that were absorbed during the day. This nocturnal operation schedule requires a sufficient amount of thermal storage capacity, but at least equally importantly, also puts requirements on the rate at which the heat storage can be charged/discharged. For effective operation of the system, it is therefore important to use a construction material with a good combination of thermal conductivity and storage characteristics. The Energy2D model was therefore also used to characterize the thermal time constant of different concrete mixtures in order to select the mixture that would be used for the initial Convective Concrete mock-up. In this study, the temperature for a point in the middle of a 20 cm thick concrete wall was simulated and the wall was subjected to a 10°C temperature step decrease. The thermal time constant, defined as the time required for this point to change $e^{-1} = 36.8\%$ of the total difference between its initial and final temperature, was evaluated for 70 existing types of concrete with different density and thermal conductivity.

Figure 3 presents all the examined concrete types according to their thermal conductivity (*x*-axis) and their density (*y*-axis). The diameter of the circle and shade of grey represents the time constant recorded during the simulation for every concrete type. The smaller and darker the dot, the shorter the time constant.

This graph provided quantitative information that allowed discussion among decision-makers and subsequent selection of a concrete mixture that has a high density for high storage capacity purposes while having a relatively quick thermal response with a time constant close to a value of 2 h, as this would facilitate a full charge/discharge during a typical day/night cycle. As can be seen in Figure 3, the selected concrete mixture has a density of 3200 kg/m³, a thermal conductivity of 2.3 W/m.K and a time constant of one hour and 56 min.
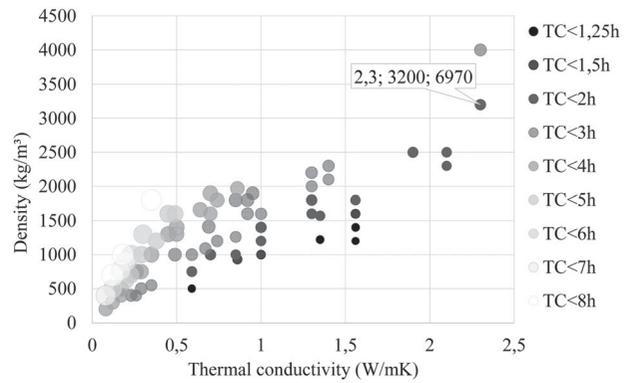

Figure 3. Thermal time constant of 70 concrete types.

3.1.3. *Whole-building simulation*

While the performance of the mock-up was being measured under controlled conditions, the timespan of the project did not allow for implementation and monitoring of the performance of the system in a real building. This situation can instead be modelled in whole building energy simulation software. No model pre-exists to simulate the innovative Convective Concrete system, however, some existing models were found to have enough similarities and flexibility to replicate the effects of Convective Concrete.

After careful consideration of the modelling capabilities in different BPS tools, it was decided to use the ventilated slab model developed by Chae and Strand (2013) in EnergyPlus as a starting point. Since the Convective Concrete does not create an airflow path between inside and outside, the 'Slab Only' mode was selected. The system is assigned to wall surfaces rather than the ceiling. Also, no heating or cooling coils were implemented as the Convective Concrete uses outdoor air directly. Heat dissipation of the fans was included in the model by assuming that all waste heat of the fan would enter the air stream. Previous studies show that, depending on e.g. building
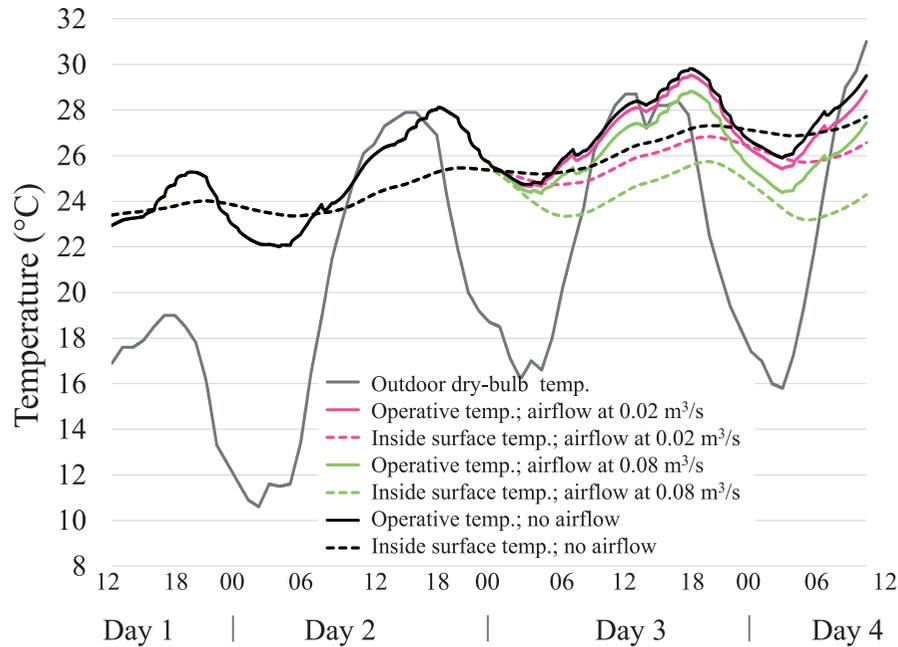
Figure 4. Effect of the convective concrete with an air flow rate of 0.02 and 0.08 m³/s compared to the system off.

type and climate, the auxiliary energy consumption for fans in comparable passive cooling systems can range from being negligible to a few kWh/day (Chae and Strand 2013; Favoino et al. 2014; Koenders, Loonen, and Hensen 2018). Since this dissipated energy consumption can play a significant role in determining the system's overall coefficient of performance (COP), it is an important factor to take into account in this type of integrated performance assessments.

Figure 4 shows the effect of Convective Concrete on a typical bedroom of 9 m² when the system starts operating on day 2 at midnight. These simulations were carried out with IWEC weather data for Amsterdam, the Netherlands. The bedroom has two walls exposed to the outside: the south wall has a window while the east wall accommodates the Convective Concrete. Other surfaces were considered to be adjacent to rooms with similar thermal conditions. The outside air was circulated in the Convective Concrete element and then released to the ambient environment. This decreases the inside surface temperature of the wall which in turn decreases the temperature of the room. The ventilation in the Convective Concrete is only on when the outside temperature is low enough to cool the element which is mostly during the night. The thermal mass of the high density Convective Concrete keeps the room cool during the day.

With this model, various system parameters were altered, and the resulting effects were visualized. In Figure 4, a low (0.02 m³/s) and high (0.08 m³/s) air flow rate were tested. As expected, the high flow rate resulted in a higher cooling effect, reducing the operative temperature up to a difference of 2°C.

The model also allowed analysis of a longer period of time and different locations. To do this with measurements would require much more time and investments. Figure 5 presents the amount of time the operative temperature in the bedroom is above 24°C from the 1st of April to the 31st of October (i.e. the period of the year in which Convective Concrete would be active), for four different locations which were derived from the climate analysis (section 3.1.4). The baseline building has a typical brick cavity wall and the same insulation level as the Convective Concrete case. While the Convective Concrete was simulated with the same low and high air flow rate as in Figure 4, the baseline building was also modelled with the possibility to use free cooling by opening the windows at night (from 10 PM to 6 AM and when the temperature outside is at least 3°C lower than the temperature inside). For all locations, a high air flow rate through Convective Concrete was required to present significant improvement of thermal comfort compared to the scenario of opening the windows at night.

3.1.4. Climate analysis

When developing a new building envelope system such as Convective Concrete, it is important to identify high-potential locations that have favourable climate characteristics with respect to the operating principles of the system. Convective Concrete is expected to work well in a climate where summer night time temperatures drop well below indoor comfort temperature. In this way, the outside air can effectively cool down the building structure, and help in reducing the extent of indoor overheating during the next
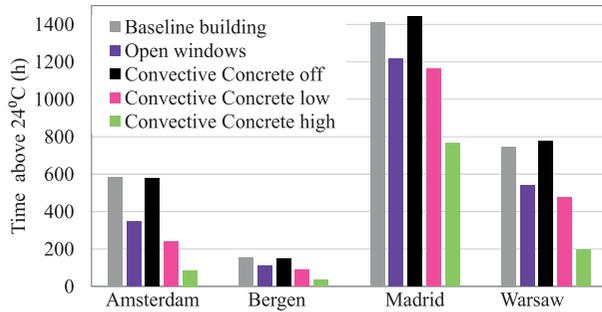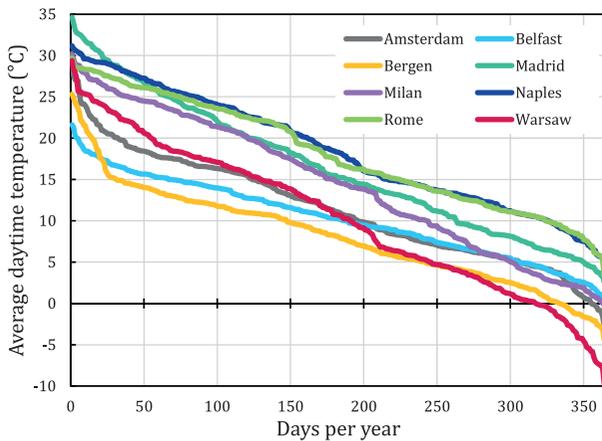
Figure 5.   Hours above 24°C for four locations.

Figure 6.   Temperature duration curves of average daytime (08h00–18h00) outside temperature.

Figure 7.   Temperature duration curves with daily temperature amplitude on the corresponding day.

day. In addition, it is important that the climate has a moderate degree of summer discomfort. The results in Figure 5 have shown that Convective Concrete is best used for peak shaving. For climates that have too little indoor overheating issues, it will be difficult to make Convective Concrete an economically viable investment. In climates that are too warm, on the other hand, buildings will likely rely on active cooling systems to ensure occupant comfort all year round.

Figure 6 shows temperature duration curves for eight European cities, inspired by the approach in Medved and Arkar (2008). These results were obtained by post-processing the information in typical meteorological year (TMY) weather files for each of the eight locations.

Each line represents the average daytime outside temperature, taken between 8 am and 8 pm. The data was sorted from high to low values to investigate the number of days per year that a certain temperature gets exceeded. The cities of Rome and Naples are considered as too warm for using Convective Concrete, since the average daily outside temperature is above 20°C for approximately half of the year. The climate of Belfast, on the other hand, has very mild summers, and consequently little need for summer cooling. The fact that both Warsaw and Madrid have continental climates, can also be observed since they both show a large temperature difference between summer and winter
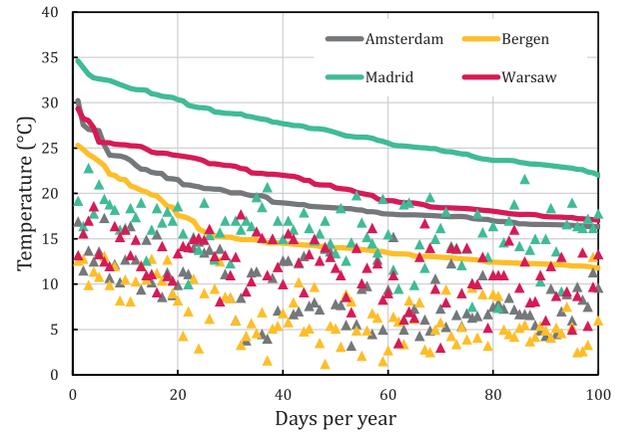
and a steep gradient. Bergen has a short, but rather intense summer season. Convective Concrete could be used to reduce indoor overheating during this period in cities such as Madrid, Warsaw, Bergen and Amsterdam.

To get a better understanding of the temperature difference between day and night, the daily amplitude in outside temperature was calculated for the four locations cited above (Figure 7). During the warmest period in Amsterdam and Warsaw, the temperature swing between day and night varies between 10 and 18°C. On some days, this is enough to get a significant temperature difference for cooling down interior spaces. There are, however, also warm summer nights in which the free cooling potential will not be enough to avoid overheating. The city of Bergen has, on average, the lowest day-night temperature difference. Still, in the summer season, this difference is mostly above 10°C, indicating that there is potential for using free cooling. Madrid experiences a climate with warm summers, but also a large temperature difference between day and night. This indicates that there is potential to use a low-energy cooling system such as Convective Concrete under these climatic conditions.

3.2.   *Case study 2 – Spong3D*

3.2.1.   *System description*

The Spong3D project investigated the potential of Additive Manufacturing to produce a façade system that integrates thermal insulation, energy harvesting, and heat storage and distribution, in addition to traditional façade requirements (Sarakinioti, Turrin, et al. 2017, 2018).

The proposed system incorporates closed air cavities which are located in the core of the façade to provide thermal insulation and has lateral channels near the outer layers which are used to circulate a liquid (water plus additive) that acts as thermal mass and heat transporting medium. Together, the composition of the channels and the cavities
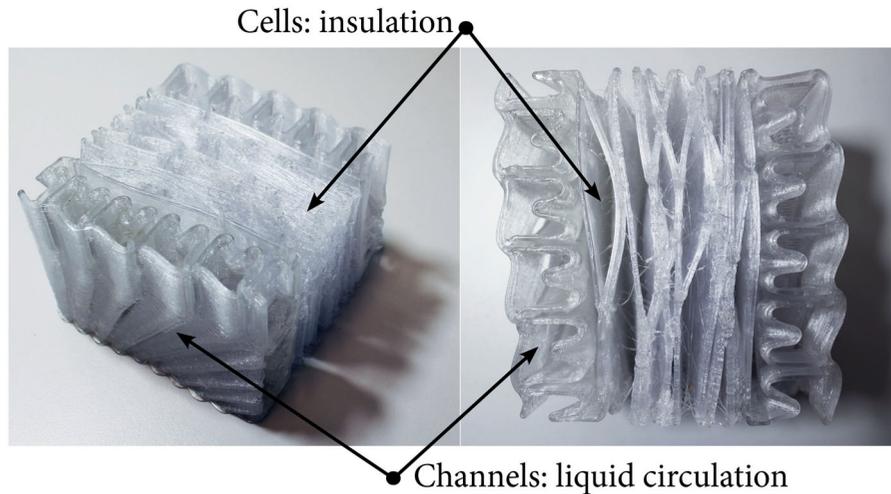
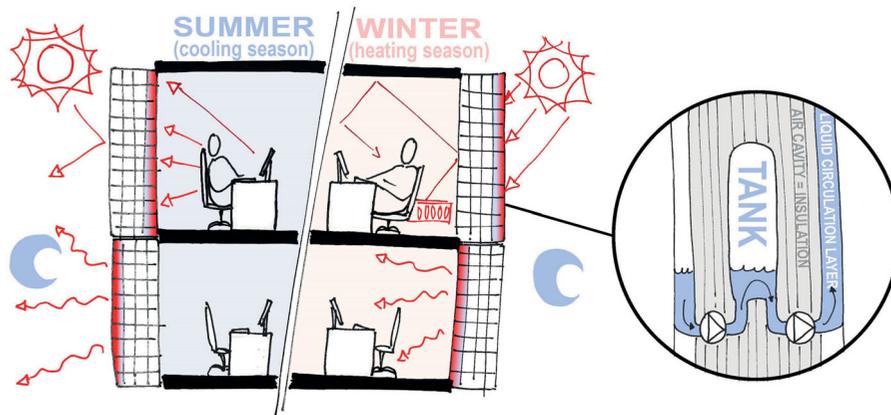Figure 8. Sample of the structure with its channels and cells.

Figure 9. Schematic illustration of the operation of the system.

form a complex structure, integrating multiple functions into a single component (Figure 8).

Two reversible pumps circulate the liquid from one side of the façade to the other, with the possibility to be stored in a tank in the middle of each façade panel when necessary (Figure 9).

In a cooling situation, the liquid is first placed on the inside to absorb internal heat gain and is then pumped to the outside layer to discharge its heat to the cool night sky. For heating purposes, the liquid is placed outside during daytime, to absorb solar heat gains and is then pumped to the inside to release this heat inside the building.

3.2.2. Simulation at the element scale

The multidisciplinary research team involved experts with various backgrounds, which ensured that every aspect of the requirements expected from the façade system was considered. In this research team, three main disciplines are highlighted: (i) design and 3D printing process, (ii) structural engineering, (iii) building physics and thermal performance. The structural engineers performed impact tests on the 3D printed material which showed unpredictable strength of the material depending on the printing conditions. The structures team expressed its concerns and suggested to apply a glass cover on both sides of the façade element to guarantee its protection. On the other hand, the design team argued that adding a glass cover would restrict the freedom of shape allowed by AM. Multiple different arguments were presented by various team members, which made it difficult to make a clear decision on which direction to continue the research. Introducing a façade system that integrates many functions with a single material and manufacturing process was one of the main goals of this project. However, the first goal was to create a façade system that integrates controlled heat exchange, storage and distribution. Therefore the decision of having a glass cover was determined based on the thermal performance of the system with and without it.

At this stage of the design, Energy2D appeared as a suitable tool to quickly assess the effect of adding a glass cover relative to not having it. The façade was modelled in section in the 2-dimentional heat transfer model. The
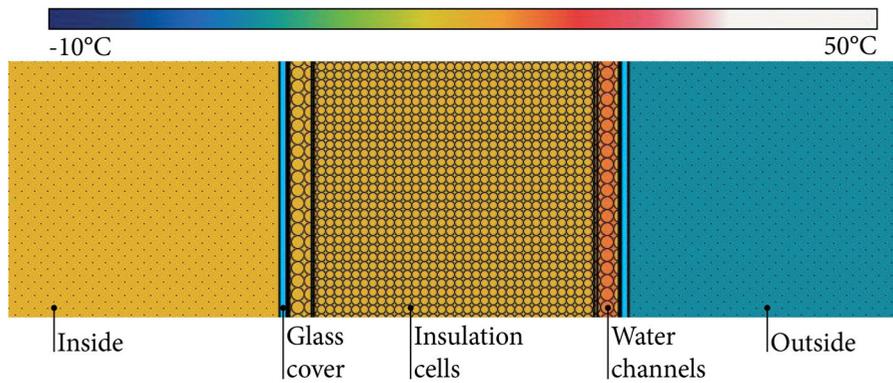
Figure 10.   Model of the Spong3D system with glass cover in Energy2D (section).
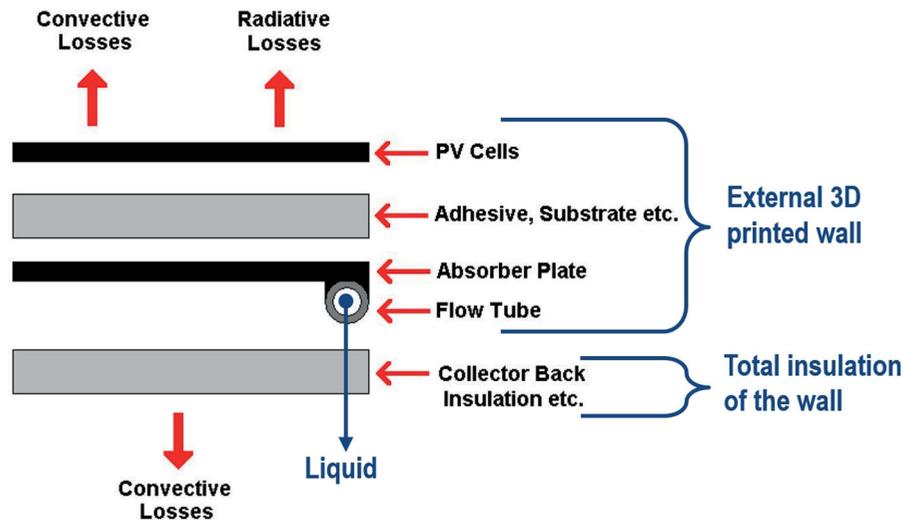

Figure 11.   Diagram model of the Spong3D system in Trnsys, which is applied as a vertical wall system. The existing PV layer of the Trnsys Type 560 was given the same thermophysical properties as the Spong3D material.

different parts of the system were modelled with layers of different properties as presented in Figure 10. The different scenarios (e.g. liquid on the outside during summer night) were tested in different models and the absorption or release of heat was studied over time.

For each scenario, the glass cover presented an extra thermal resistance which reduced the release or absorption of heat by the liquid layer in the first 10 h after a temperature step change. These simulations allowed quantitative results to be quickly produced, leading to actionable information that allowed the research team to move on in a common direction.

3.2.3.   *Whole-building simulation*

Similarly to Convective Concrete, as explained above, the behaviour of the Spong3D system cannot be captured with any existing model from a whole-building simulation programme. However, the water layer on the outside operates in a similar way to a solar collector. It absorbs heat from solar radiation during sunny winter days and exchanges the thermal energy to a liquid with a specified mass flow

rate. The same model can be used to investigate heat losses during cool summer nights.

As explained previously, the solar collector model should be unglazed to reduce the resistance to heat transfer. Therefore, the component Type 560 in Trnsys was used. It models a combined PV/T solar collector. As shown in Figure 11, the properties of the flow tube, absorber plate, adhesive, substrate and PV cells are modified to represent the properties of the 3D printed water channel wall which has a thermal resistance of $0.0092\,m^2\,K/W$. The Spong3D concept does not comprise a PV layer. By adjusting thermophysical properties of the PV layer to meet the characteristics of Spong3D, and setting the PV conversion efficiency to 0%, it was ensured that the PV functionality of the original model would not have any negative consequences for the performance prediction of Spong3D.

The focus of the simulation presented here is on the summer night and winter day scenarios when the liquid is placed on the outer channels and interacts with the outside climatic conditions.

The weather file used in this simulation (IWEC weather file, Amsterdam, The Netherlands) allows to observe the
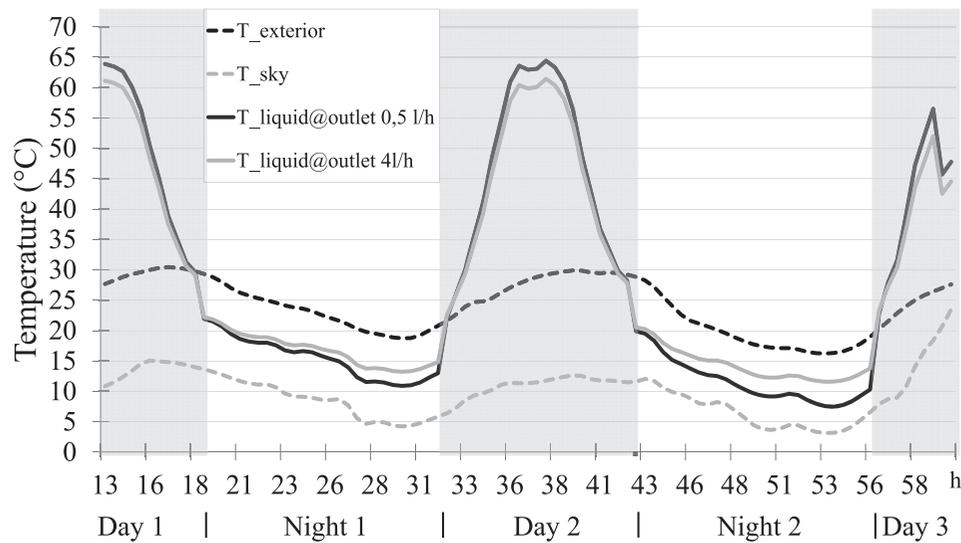
Figure 12. Trnsys results showing the temperature of the liquid during two summer nights for two mass flow rates.

dynamic effects of the climate on the temperature in the channels. Until now, the different scenarios of the liquid being placed in the inner or outer channel layer were looked at separately. But the result of one simulation can also be used as input for the other. This model allows to alter various parameters such as: thermal properties of the front cover, mass flow rate of the liquid, thermal properties of the liquid, outside climate conditions.

Figure 12 shows that a lower mass flow of 0.5 l/h releases more heat during the night than a high flow rate of 4 l/h. A similar trend was observed for the scenario of a sunny winter day where a low mass flow rate of the liquid allows it to get warmer than with a high mass flow rate.

In a later stage of the project, annual simulations were carried out with a TRNSYS model in which all components for absorbing, storing and releasing thermal energy were fully coupled. The interested reader is referred to Sarakinioti, Konstantinou, et al. (2018) for more details.

3.2.4. Climate analysis

As mentioned in section 3.2.3, the system can be tested under different climate conditions. But simply investigating the weather files (e.g. TMY), without performing the actual simulations can also give useful cues about the prospective performance of the system in different locations.

As seen in Figure 12, the outside temperature, but more importantly the sky temperature will determine how easily the heat in the liquid will be released to the environment at night during the summer. In winter, it is important to look at the outside temperature and at the solar radiation since the Spong3D system would work best in locations with cold but sunny winter days. Figure 13 presents four colour maps created with the Ladybug plug-in for

Grasshopper (Sadeghipour Roudsari and Pak 2013). Each pixel represents one hour of one winter day and is coloured according to the legend on the right. Data was obtained from the IWEC file for Amsterdam, the Netherlands, and the CWEC file for Toronto, Canada. The top chart shows the solar irradiance between 200 and 1000 Wh/m^2 and the second from the top shows the dry-bulb temperature from -10 to 20°C, both for Amsterdam, the Netherlands. The two bottom charts show the same but for Toronto, Canada. In Amsterdam, the global horizontal irradiance (GHI) in winter months from December until February reaches values above 250 W/m^2 for 6.8% of the daylit hours, while ambient temperatures above 5°C were recorded during 47.5% of the time. In the same period in Toronto, ambient temperatures higher than 5°C only happen for 2.9% of the time, but in this climate, the occurrence of clear skies is much higher, as indicated by the fact that GHI values above 250 W/m^2 are present for 24.3% of the daylit hours. Because the potential contribution of Spong3D towards reducing heating energy demand in winter is largely determined by the availability of direct solar irradiance, its application is most promising in Toronto. It is likely that a different conclusion would have been reached if only traditional heating degree days (HDD) would have been considered, with HDD = 3956 for Toronto and HDD = 3038 for Amsterdam (ASHRAE 2009).

3.3. Case study 3 − Tunable IR-reflective glass

3.3.1. System description

This study investigates the performance of an innovative switchable window coating that selectively transmits/reflects near-infrared sunlight. In a previous simulation study, the impact of such windows on heating and cooling energy consumption and thermal comfort
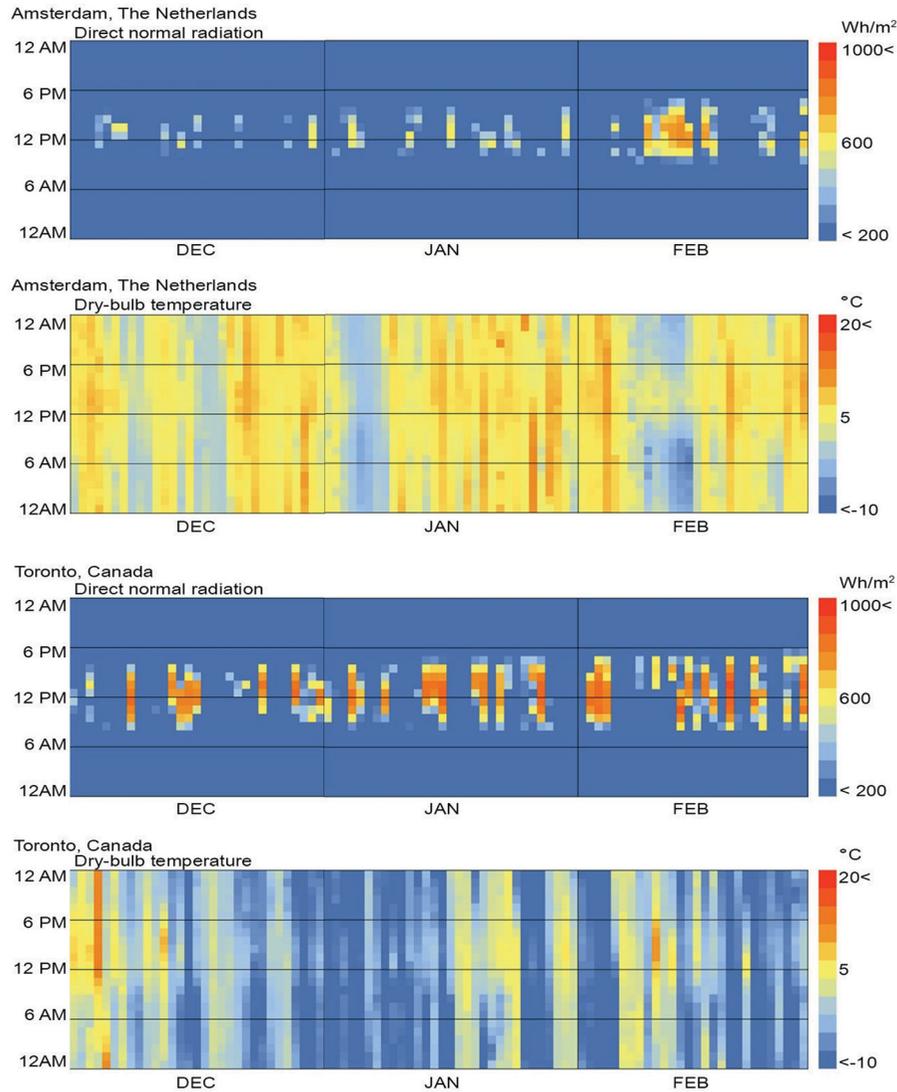
Figure 13.   Radiation and temperature flood chart for Amsterdam (top) and Toronto (bottom).

in buildings was already investigated (Khandelwal et al. 2015). During that project, it was identified that the performance of switchable NIR (near-infrared) reflecting coatings can be further improved by increasing the difference in solar-optical properties between (i) the neutral/transparent state, and (ii) the reflecting state of the window. Considering the spectral transmittance of the responsive layer, the difference between these two window states can be increased in two ways (Figure 14):

- A: Increasing the depth of the reflection band by interacting with both left-handed and right-handed circularly polarized light.
- B: Increasing the width of the reflection band to interact with light in a wider part of the solar spectrum, by (i) choosing the right concentration of chiral dopant, and (ii) tuning the photo-polymerization process.

The focus of this study is on investigating the potential of approach B. From Figure 15, that shows the spectral intensity of sunlight, it is clear that extending the reflection band towards the direction with lower wavelengths has the highest potential due to the higher intensity of sunlight in that region. However, when the cut-off wavelength, defined as the sharp edge of the reflection band, gets too close to the visible range, there is a risk for unwanted visible disturbance. This disturbance consists of pink/red window colouration, caused by photometric reflectance under certain incident angles. The present design of the NIR reflecting window film introduces a safety margin to avoid the risk for this kind of visible interference. From an energy-efficiency perspective, this safety margin represents a missed opportunity. It is currently unclear what the added value of shifting the cut-off wavelength closer to the visible range would be, and whether such benefits could potentially outweigh
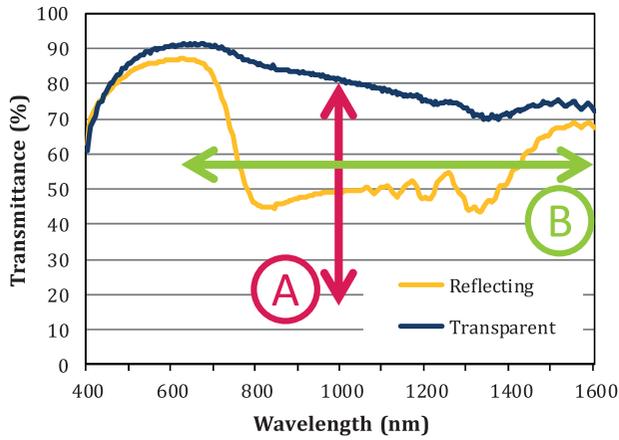
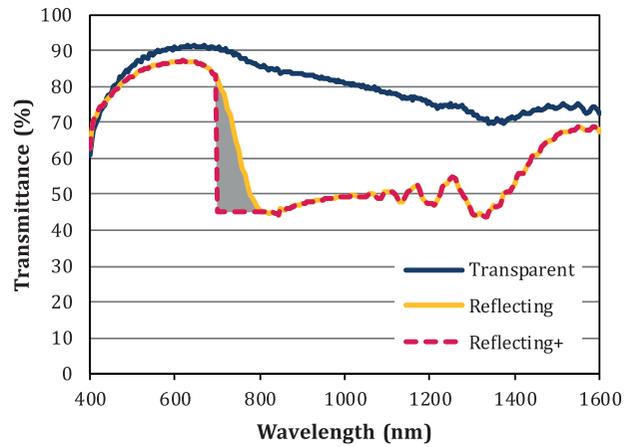Figure 14. Spectral transmittance of the switchable NIR reflecting layer.

Figure 16. The reflecting + film has a sharp cut-off wavelength at 700 nm.

the risks and drawback that come from visible colouration.

3.3.2. Simulation at the element scale

In this study, we assume the spectral window properties as given in Figure 16. The cut-off point for this window prototype is not very steep. Instead of a single point, it actually corresponds to a transition range, roughly between 700 and 800 nm. To evaluate the impact of enhanced wavelength cut-off, we assume that it is possible to fabricate the ideal case with a steep cut-off point at 700 nm (red line in Figure 16, referred to as 'reflecting +' state).

The difference in transmittance between the reflecting and reflecting + state is represented by the grey area in Figure 16. Solar transmission properties at normal incidence angle of the three glass layers were calculated with

Table 1. Solar-optical properties of the three window states.

	T_{sol}	$T_{non-vis}$
Transparent state	0.82	0.83
Reflecting state	0.70	0.53
Reflecting + state	0.67	0.48

respect to the ASTM G173-03 reference solar spectrum (Table 1), where T_{sol} indicates the whole solar spectrum, and $T_{non-vis}$ only the wavelengths between 701 and 4000 nm.

Based on the ASTM G173-03 spectrum, 13.1% of the sunlight is active in the wavelength range between 700 and 800 nm. Compared to the spectral properties of the current-generation window (i.e. reflecting state), Table 1 shows
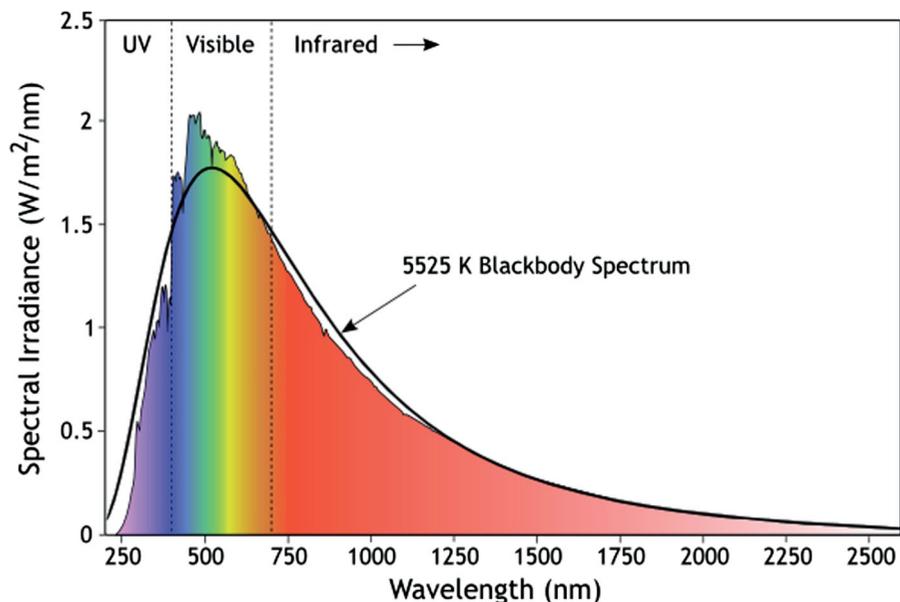

Figure 15. Spectral irradiance of sunlight.

that an extra 5% of non-visible reflectance can be achieved with the idealized reflection cut-off point (i.e. reflecting+ state). When integrating this behaviour over the whole solar spectrum, the total solar transmittance reduces from 70% to 67%.

3.3.3. Whole-building simulation

The extra benefit of this increased reflection on building energy efficiency was evaluated, by inputting these new window properties into a whole-building simulation model. TRNSYS Type 56, with its two-band solar radiation model was used to analyze the performance. Glazing properties were obtained through measurements and calculations, and inserted in the LBNL Window7 program (LBNL 2017). The switching between the different glazing states was achieved by changing the glazing id-number through a signal from Trnsys Simulation Studio during simulation run-time. For the simulations that are reported here, the same assumptions and window control strategies were used, as reported in Khandelwal et al. (2015). The results in Figure 17 show that for a South facing office in the climate of Madrid, an extra reduction of 15% of the cooling energy demand is possible with the additional reflection in the range between 700 and 800 nm. In these simulations, it is assumed that the window switches from the reflecting to the transparent state when the indoor operating temperature gets lower than 22°C during daytime.

Due to the high intensity of sunlight in the wavelength range just outside the visible region, it appears worthwhile to explore if reflectivity of the NIR coating in this range can be improved. The current study, which assumed idealized reflection properties in this range, shows that an additional 15% of cooling energy reduction is possible. This finding appears to warrant more R&D efforts that aim at fabricating NIR reflecting films with such properties. However, more combined qualitative and quantitative research, especially regarding perception studies with large prototypes, is still needed to evaluate how this extra energy-saving potential would weigh up against possible disturbance in terms of pink/red window colouration effects.

4. Discussion and conclusions

4.1. Main findings

Literature shows that BPS has occasionally been used to support decision-making in product development of innovative building envelope components in industry. It was found, however, that its application in more explorative projects, such as the ones reported in this article, is rare, whereas a discussion of modelling issues and process integration challenges that goes beyond the analysis of individual application examples is missing in the scientific literature. A perceived mismatch between simulation capabilities and the need for rapid feedback in relation to the ill-defined and evolving nature of explorative R&D

projects is believed to inhibit the use of BPS in these explorative contexts. Among the challenges are the occurring trade-offs between model complexity and accuracy, the absence of suitable component models, ways of dealing with incomplete or uncertain data, and the need to present results in a concise yet informative way.

The various short simulation studies presented in this paper, which were deployed in response to the needs posed by different questions in multiple phases of the R&D process, however, have shown that the application of a range of complementary BPS approaches has potential to overcome some of the challenges, as it has been demonstrated that this can provide valuable feedback to R&D teams, by:

- Providing quick estimates about the performance of multiple problem-solution pairs to offer early information that helps choosing among different development directions.
- Giving the R&D team the opportunity to analyze the energy and comfort consequences of their decisions at multiple spatial scales, from material to whole-building level. The dynamic features of BPS are especially relevant, because due to the high influence of thermal inertia, simple calculation methods and rules-of-thumb may not suffice.
- Enabling the option to conduct virtual experiments and explore what-if scenarios (e.g. different climate conditions or control strategies) in a quick and cost-effective manner.
- Helping in the definition and design of physical experiments that use available resources efficiently.
- Allowing for the exploration of the performance of materials and components with not-yet-existing properties. This is, evidently, not possible in experimental research.
- Confirming engineering intuition by means of quantitative metrics. Or alternatively, providing physics-based insights in situations where counterintuitive effects are to be expected.

With the use of BPS, it is possible to perform early-stage tests that would normally only be possible at much higher technology readiness levels. In this way, resource efficiency in the R&D process is promoted, and the time to market can potentially be shortened. Similarly, the deployment of BPS can also lead to timely termination of a project, in cases where it is determined that even in an optimistic scenario, the potential benefits of the system would not outweigh the costs. This type of information is not only helpful for making informed decisions when selecting between different design alternatives, it may also help in determining the longer-term outlook of the innovation. For example, simulations can provide quantitative input for business models and identification of high potential niche markets, it can provide substantiated arguments in discussions about added value versus lowest cost (Loosemore and
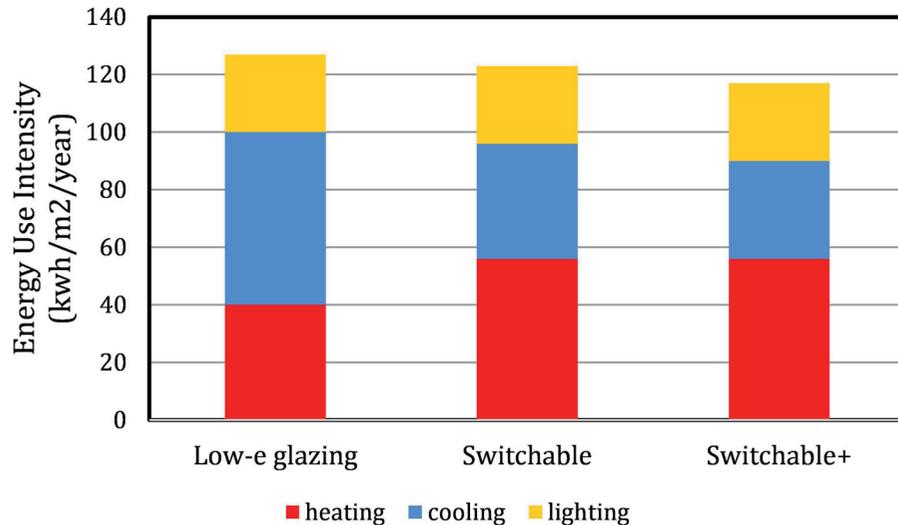
Figure 17. Comparison of the energy-saving potential of (i) a reference glazing system (low-e), (ii) the current generation NIR-reflecting switchable glazing system, and (iii) the NIR-reflecting switchable window with enhanced spectral properties.

Richard 2015), as well as realistic projections for attracting possible follow-up funding.

We have also demonstrated that systematic analysis of datasets with typical meteorological weather data can lead to additional useful insights. Although the use of TMY files is strictly speaking not a simulation activity, it is closely related to the building simulation field, and therefore also considered in this paper. More pervasive use of this type of climate analysis is recommended, since it facilitates easy targeting of most promising application areas, and tuning of design specifications in response to these conditions.

Dealing with first-of-its-kind innovative façade concepts often means that the tools available for simulations on the whole-building scale do not have sufficient modelling capabilities to support performance evaluation of these specific elements. It should be noted, though, that many simulation models can be reused outside their initially intended application domain, as long as there is sufficient attention for quality assurance. Using examples of the ventilated slab in EnergyPlus, and a BIPVT collector in Trnsys, this paper has demonstrated two examples of such a creative use of legacy simulation software.

4.2. Points of attention and recommendations for users and software developers

Literature in the fields of operations research and management studies is rife with articles that provide guidance about how to avoid misuse of modelling and simulation (Banks and Chwif 2011; Chwif, Barretto, and Paul 2000; Law and McComas 1991; Uhrmacher 2012). Many of the principles that are presented in those papers do also apply to the field of building performance simulation, and are particularly relevant considering the challenges that arise from its use in explorative R&D contexts.

One ought to be reminded that the use of simulation is not a silver-bullet solution. In the first place, it should be ensured that sufficient resources (time and budget) are available to be able to accomplish the expected tasks. Sufficient domain knowledge of the simulation user is indispensable and an often underestimated factor when considering quality assurance of simulation studies (Hensen 2004). Moreover, it is important to educate the decision makers and other team members about what is realistic and possible when aiding the solution-finding process with simulations. Due attention should be paid to intelligible visualization of the results (Bleil de Souza and Tucker 2014), as it has been demonstrated that sensory and perceptually effective presentations can significantly enhance the communication opportunities with non-simulation-experts (Hamza and De Wilde 2014). When not all of the conditions above are met, it is probably wise to abstain from embarking on simulation studies at all (Banks and Gibson 1997).

Another important point of attention to be aware of is the complexity pitfall (Banks and Chwif 2011). In early phases of the R&D project, the simulation models likely need to be developed in an information-poor context. Considering the trade-offs between abstraction error and the uncertainty that comes with estimation of unknown or undecided parameters, it is a common risk to develop models that are overly complex (Chwif, Barretto, and Paul 2000; Gaetani, Hoes, and Hensen 2016). Such models do not only waste development time and computational resources, but more importantly, can also compromise the quality of the predictions. Rather, one should aspire to match the type and resolution of the model to the specifics of the stakeholder and the task at hand. When developing such fit-for-purpose models in an evolving environment, it is wise to develop hierarchic models, such that previous efforts can be reused (Wetter 2011).

Based on the findings described above, developers of BPS software are encouraged to consider the following features in next generation simulation tools to better cater for the needs of users who use BPS in explorative R&D contexts:

- Provide capabilities for efficient visualization of weather files and associated analyses such as the ones presented in this paper.
- Allow for modular and hierarchic model formulations that can co-evolve with the technology readiness level of the concept and the information that becomes available.
- Provide access to the source code and information about underlying assumptions.
- Develop new approaches for results visualization, at different temporal and spatial scales, to be used for effective communication with various groups of stakeholders.
- Extend possibilities for testing the performance of different control strategies, which is currently one of the main limitations in performance prediction of advanced facades (Loonen et al. 2017).
- Integrate simulation models with sensitivity analysis and uncertainty propagation techniques to assist the R&D team in prioritizing important design variables and to reach robust final products.

4.3.   *Future trends*

To be able to respond to ever stricter environmental policies, while accommodating the health and well-being aspects of buildings with high environmental quality, there is a growing need to devise innovative façade concepts, systems and materials. It is expected that the use of BPS can co-benefit from other automation trends in the construction industry to expedite this transition.

Two of the projects that are discussed in this article make use of additive manufacturing as a production method for making prototypes as well as the final product. The application of AM as a rapid prototyping tool has led to many design iterations and a strong mutual interaction with simulation activities. With the growing interest in AM and other digital production techniques in the construction industry (Kothman and Faber 2016), we also foresee many promising opportunities to further take advantage of the coupling with BPS.

There are several other trends in the field of computational building performance analysis, such as generative and parametric design methods, enhanced simulation domain integration (e.g. thermal, visual and airflow), advanced visualization techniques and the use of building information modelling. It is expected that these developments will help in further reducing the barrier for applying BPS in exploration-driven R&D projects.

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