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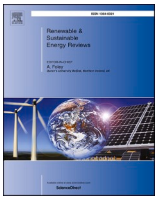

A narrative review to credible computational fluid dynamics models of naturally ventilated built environments

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ABSTRACT

This narrative review describes the capabilities of computational fluid dynamics (CFD) to support the scientific analysis of fluid flows inside buildings, focusing on natural ventilation. The challenges posed by CFD, such as mesh generation, boundary conditions specification, choice of turbulence or radiation models and the ability to estimate the accuracy of results are explored. For the first time, this work provides a summary of verification and validation studies relating to CFD models of different built environments, and detailed validation studies of naturally ventilated spaces. This review summarises the most common guidelines and conclusions drawn from literature relating to CFD modelling of indoor environments that are naturally ventilated.

The work demonstrates current practices in CFD simulation of naturally ventilated indoor environments, highlighting the importance of quality assured validation data to support the credibility of models. The review shows that, despite the presence of best practice guidelines for verification and validation of computational models, the grid verification was infrequently reported in the literature when presenting CFD results of indoor environmental conditions. Moreover, a third of reviewed validation studies were only qualitative and lacked specific validation criteria.

Credible CFD analysis of natural ventilation strategies in buildings requires the ability to interpret strongly variable field measurements when specifying boundary conditions, other computational parameters and validating model results. This research provides a background and general guidelines for researchers who are commencing work in the field of CFD simulation of indoor environments for flow problems relating to natural ventilation.

1. Introduction

Computational fluid dynamics (CFD) is a modelling approach that uses numerical methods to describe phenomena involving fluid flows to a high spatial and temporal detail. CFD is widely used in many modern engineering fields. Starting from applications in fields of aeronautics and astronautics, through process, chemical and biomedical engineering, including civil and environmental engineering; CFD provides the technical basis for improving new and optimising existing designs. This results in higher process efficiency at a lower cost. By producing detailed information about the fluid flow, heat transfer and contaminant concentration, CFD has become more common as the choice of technology in performance modelling of internal and external built environments. This is supported by the fact that, over the last 60 years, CFD has progressively become more accessible for research and industry sectors, mainly because of the development and advancement in computing processing power and the availability of commercial software. In spite of the user-friendly interfaces and simplicity of use of the commercial codes (when compared to the academic codes), it is essential to ensure that CFD results are realistic [1].

According to the International Energy Agency, in 2021 the operation of buildings was responsible for 30 % of global final energy consumption [2]. Half of the energy consumed by buildings is due to the use of

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Abbreviations

ASHRAE -	American Society of Heating, Refrigerating and Air-Conditioning Engineers
BMS –	building management system
CFD –	computational fluid dynamics
DES –	detached eddy simulation
GCI –	grid convergence index
HVAC –	heating, ventilation and air conditioning
LES –	large eddy simulation
RANS -	Reynolds-averaged Navier-Stokes
RNG -	renormalization group
SDG –	sustainable development goal
SST –	shear stress transport
URANS –	unsteady Reynolds-averaged Navier-Stokes

heating, ventilation and air conditioning (HVAC) systems [3]. Thus, it is very important to provide safe, healthy and comfortable conditions in buildings (which incorporate living and working environments) that require minimum energy demand.

Natural ventilation is a sustainable solution to maintain healthy and comfortable environmental conditions in buildings. However, an effective design of naturally ventilated spaces requires a good understanding of the complex airflow patterns caused by buoyancy and wind effects and unique nature of buildings' geometry. Thus, without the proper tools to capture, predict and optimise the environments in naturally ventilated buildings, the provision of healthy and comfortable conditions for the occupants cannot be guaranteed with any degree of confidence.

Previous research investigated the suit of options and approaches available for building performance analysis, including building energy balance models, zonal airflow network models and CFD among others, e.g. Refs. [4,5]. The choice of an appropriate simulation approach depends on the problem investigated and implies different levels of results' accuracy and simulation costs [4]. When compared to other methods (e.g. analytical and experimental) for predicting ventilation performance in buildings, CFD was found to be very popular, with studies seeking more accurate and reliable CFD models [6]. While airflow network models predict airflows between different zones in a building and the outside (each zone represented by a zone temperature, pressure and possibly contaminant concentration) [7], CFD could also provide the most detailed information about the performance of ventilation systems in a particular zone (e.g. temperature stratification, air velocity and direction, contaminant dispersion), provided the model is created by a user with solid fluid dynamics knowledge and validated with experimental data [5].

The accuracy and reliability of the CFD predictions remains a big concern (e.g. Refs. [8,9]). A converged CFD simulation does not necessarily mean a correct solution. The accuracy of the CFD results depends on the modeller's knowledge of fluid dynamics, the expertise to handle complex boundary conditions (and the quality of that information) and skills in numerical techniques (e.g. Ref. [10]). Many types of errors and uncertainties may arise during the development of a CFD simulation. Thus, close attention must be given to the development and verification of a computational model, as well as utilisation of trusted experimental data for model validation.

Previous research [11] indicated a need for comprehensive studies that systematically guide, explain and ensure credibility of CFD simulations of naturally ventilated built environments. Thus, the aim of this narrative review is to answer the question of how to achieve credible CFD models of naturally ventilated indoor environments. Attention is given to ventilation through openings and not specifically designed natural supply/exhaust grilles. However, some studies concerning mechanical ventilation in buildings are also mentioned when discussing the flow and boundary problems and validation/calibration studies.

The literature review focuses on two main and novel objectives. The first objective is to provide a summary of verification and validation studies relating to CFD models of different built environments, and detailed validation studies of naturally ventilated spaces. The second objective is to generate an original summary of the most common guidelines and conclusions drawn from literature relating to CFD modelling of indoor environments in combination with natural ventilation.

The research summarises literature under the main topics of natural ventilation and credibility of CFD simulations. This is done to provide the readers with technical knowledge, supported by applications and case studies, of investigating natural ventilation in buildings with CFD. The work is novel as it provides literature background for researchers who are commencing work in the field of CFD modelling of naturally ventilated indoor environments. The narrative review results in a solid summary of verification and validation methods for CFD simulations, highlighting the importance of quality assured data to support the credibility of computational models. Finally, the review proposes the most common guidelines and conclusions drawn from literature relating to CFD modelling of indoor environments.

The narrative review methodology included extensive searches for pivotal publications in the area of CFD model development, verification, validation and calibration, and natural ventilation in built environments. This primarily included original and review papers, but also standards and best practice guidelines for verification and validation of computational models published before 2023. The literature search focused on databases such as Scopus, Web of Science and Google Scholar. The initial selected keywords included 'computational fluid dynamics', 'CFD', 'buildings', 'indoor environment' and 'natural ventilation'. Next, the search focused on the credibility of CFD models, and the keywords of 'verification', 'validation' and 'calibration' were selected. Some examples of search strings included ('CFD' OR 'computational fluid dynamics') AND 'natural ventilation'; ('CFD' OR 'computational fluid dynamics') AND ('validation' OR 'verification' OR 'calibration'). In some cases, the snowball method was used where key publications in the field were used to identify further literature on the topic.

The review is structured in such a way to 'bring' the reader on a journey towards credible CFD models of naturally ventilated built environments. Section 2 focuses on methods, including natural ventilation, indicating the drivers and barriers to implementing this strategy in buildings; and CFD as a simulation approach that enables a detailed investigation of indoor environmental conditions in buildings. Section 3 focuses on the results of this narrative review, i.e. necessary steps to develop a trusted CFD model of an indoor environment, including mesh generation, flow and boundary conditions, turbulence and radiation models, and selection of a simulation type. This section also guides the reader on the practices for verification, validation and calibration of CFD models. Finally, Section 4 concludes with a discussion and a summary of the most common guidelines for credible CFD models of naturally ventilated built environments.

2. Methods

2.1. Natural ventilation

The use of natural ventilation can be an effective solution to save energy in buildings in the intermediate and cooling seasons. Furthermore, well-planned natural ventilation systems provide fresh air movement, which leads to comfortable and healthy indoor conditions. However, an effective design of a naturally ventilated space requires a good understanding of airflow patterns inside and outside the building [12].

Fig. 1 shows different natural ventilation strategies for a building.

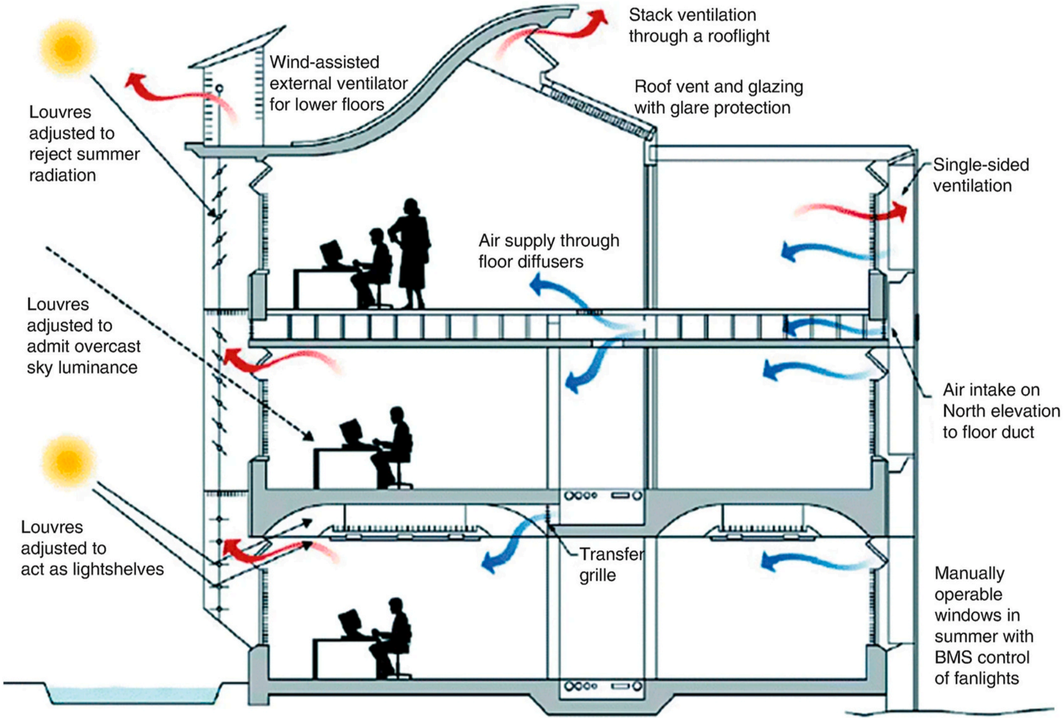

Fig. 1. Schematic of different natural ventilation strategies [18].

Buoyancy-driven ventilation prevails in many naturally ventilated buildings, i.e. where airflow is caused by pressure differences across the building. The pressure differences are, in turn, caused by air density differences, which are due to temperature differences. The effectiveness of buoyancy-driven ventilation depends on the building geometry, size of inlets/outlets, height of the space, strength of heat sources, driving the temperature difference between indoor and outdoor spaces, and as a result of that the airflow [13]. Wind-driven ventilation is influenced by highly unpredictable wind speed and direction. Generally, the design of buildings with wind-driven ventilation is based on mean wind speeds over a specific period of time [14]. The combination of these two ventilation approaches is a new trend and a challenging strategy for free space cooling in buildings [15]. According to opening locations, natural ventilation is also commonly categorised into four strategies: cross ventilation, corner ventilation, stack ventilation and single-sided ventilation [16]. Natural ventilation systems should be designed to meet the main requirements of building environmental performance. Firstly, the ventilation system must maintain adequate levels of indoor air quality. Secondly, the ventilation system should (in combination with other measures) reduce the building's tendency to overheat, particularly in summer [17].

There is an increased demand for natural ventilation solutions, from both an economic and social point of view. A fresh air movement in buildings results in high occupant satisfaction, improved health and well-being, which, in turn, can lead to increased creativity and productivity, and lower work absenteeism [19]. Natural ventilation generates more engaged building users, who are aware of indoor environmental conditions, have larger comfort temperature tolerance [20] with the capability to control ventilation themselves. For instance, the adaptive comfort theory, now included in American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) Standard 55, "*has become the global standard for designing and operating naturally ventilated buildings and has led to energy savings worldwide*" [21].

On the other hand, natural ventilation meets many barriers before it can be implemented in buildings. Natural ventilation meets practical and social resistance, it can be perceived too risky by architects and designers (when compared to mechanical ventilation) [22] and requires a change in mindset in industry accustomed to mechanical ventilation. Some studies stated that although natural ventilation can be an energy-efficient approach to improve indoor air quality, it should be supplemented in some cases with appropriate mechanical ventilation ([23,24]). Additionally, building laws are not too permissive regarding natural ventilation in some cases since the installation of mechanical ventilation is compulsory in some buildings [25].

In the end, an effective design, operation and retrofit of naturally ventilated spaces require a good understanding of complex airflow patterns caused by buoyancy and wind effects. Thus, without adequate tools to predict and optimise environments in naturally ventilated buildings, the provision of healthy and comfortable conditions for occupants cannot be guaranteed with any degree of confidence. There are no 'off-the-shelf' solutions for natural ventilation. Designers must consider different factors when proposing natural ventilation; many of these factors are not as critical in mechanically ventilated buildings [26]. There are restrictions regarding building location and orientation, outdoor conditions (wind patterns, air quality, noise, etc.) and fire safety when planning naturally ventilated buildings.

2.2. *Computational fluid dynamics (CFD)*

There exists a significant challenge to create quality simulation models that can predict the performance of naturally ventilated spaces and demonstrate compliance with environmental standard requirements. Such simulations must enable acceptable thermal performance of naturally ventilated buildings, through the design and optimisation stages [27].

With the abundance of simulation approaches available to predict and optimise building performance, the choice of the right one for a particular airflow problem is important. Previous research [4] developed a guideline for selecting a simulation approach for airflow prediction. The work indicated that CFD was the most suitable approach for investigating comfort related building performance, particularly local discomfort, turbulence intensity and local mean age of air. Thus, credible CFD simulation can provide a detailed view of how temperature, airflow, occupants, building materials and systems (including contamination sources) can impact the quality of indoor environment in a room. In relation to natural ventilation, CFD can help in estimating how the parameters of the external airflow influence indoor environment in buildings, e.g. Refs. [28,29].

Previous research utilised CFD to study wind-driven indoor airflow depending on outdoor conditions, such as wind speed/angle (e.g. Refs. [30,31]) and ambient temperature [32]. The wind interactions at different building sites were investigated previously [33] in terms of natural ventilation, to improve the selection of future sites for natural ventilation purposes. Moreover, the influence of inlet geometrical conditions, such as opening configurations, has been investigated, e.g. Refs. [34–36]. In case of buoyancy-driven ventilation, CFD simulations are particularly sensitive to the specification of boundary conditions [12]. Hence, validation procedures, supported by modelling guidelines, are required to successfully simulate the nature of buoyancy-driven flows [37]. The buoyancy effects are induced by differentials in temperature between indoors and outdoors. Previous CFD research has widely described buoyancy phenomena occurring in street canyons (e.g. Ref. [38]), whole buildings (e.g. Refs. [32,39]), rooms (e.g. Refs. [40,41]) or cavity walls (e.g. Refs. [42,43]). Moreover, recommendations regarding turbulence modelling in CFD analysis of naturally ventilated spaces have been previously provided. For instance, Zhang et al. [44] used Reynolds-averaged Navier-Stokes (RANS) approach and large eddy simulation (LES) to model both single-sided naturally ventilated spaces and cross-ventilation and concluded that LES showed better agreement with the experimental data but at a higher computational demand. Furthermore, Horan and Finn [45] found standard k-ε and k-ω turbulence models performed well in predicting airflow in a naturally ventilated building. Moreover, Jiang and Chen [46] showed that standard k-ε turbulence model could model detailed airflow distribution inside a single sided naturally ventilated room and required less computing time than the LES model. The renormalization group (RNG) k-ε turbulence model also proved to be accurate when modelling ventilation rates and air distribution inside a room with a wind driven natural ventilation [47]. A LES approach, based on leveraging the weak imposition of Dirichlet boundary conditions and on the residual-based variational multiscale method, was recently deployed with success to simulate natural driven ventilation in full-scale building with complex geometries [48]. Thus, such approaches, which employ wall functions to reduce computational efforts in boundary layers, can be promising to simulate more real and complex flows.

In the case of natural ventilation, boundary conditions and indoor environmental data are field dependent and, thus, strongly variable. The buoyancy and wind effects might generate very complex airflow patterns; hence, modelling this type of ventilation systems may be problematic [49]. Furthermore, even simple geometry CFD models, in the case of natural ventilation, may produce misleading results [50]. For these reasons, CFD analysis of natural ventilation in built environments requires CFD expertise, quality assured validation data (measured with reliable and calibrated equipment, with experimental error taken into account) and should follow the systematic procedure to obtain a reliable model of environmental conditions in a real building [28]. A perspective on the past fifty years of natural ventilation research [22] showed that more research was warranted into the operation of naturally ventilated and 'intelligent' buildings.

3. Results

This section presents the results of the narrative review focusing on the steps to achieving credible CFD models of naturally ventilated built environments.

The development of a reliable CFD simulations is challenging. Verification and validation can enable the credibility of engineering predictions and, thus, reduce the time, cost and danger associated with

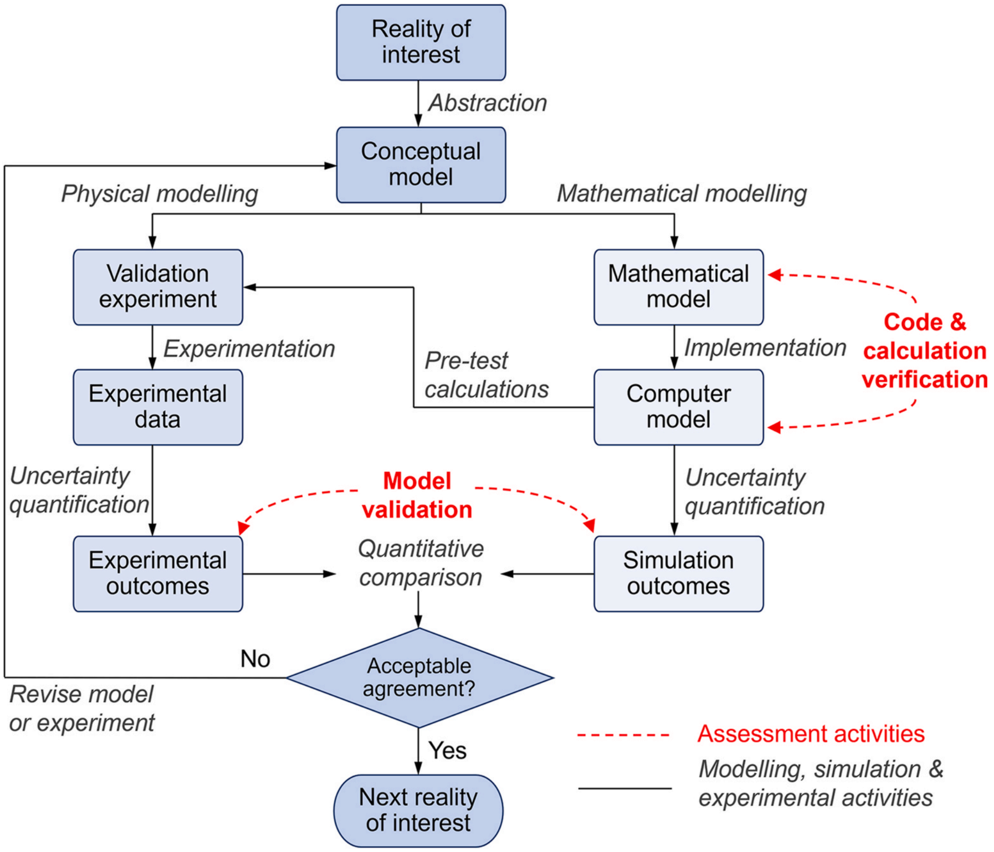

Fig. 2. Steps to the development, verification and validation of engineering models, redrawn from Ref. [51].

component and full-scale testing of products or systems. Fig. 2 shows a detailed development, verification and validation of engineering models proposed by Thacker [51]. When creating a simulation model (i.e. mathematical model) that is to represent a reality of interest, different stages of verification are required in order to estimate the performance of the simulation model. Those stages include code and calculation verification (within the mathematical model itself) and model validation, when comparing the simulation and trusted experimental (from the physical model) outcomes.

The terminology for verification, validation and calibration in CFD simulations was clarified by the American Institute of Aeronautics and Astronautics [8] and is explained in the later sections of this work. Two comprehensive studies provided clear guidance for verification, validation and reporting of the results for CFD simulations of indoor environments ([52,53]). Many additional guidelines, on how to generate credible (i.e. verified and validated) CFD models in general, have been developed (e.g. Refs. [54–57]), followed by the studies analysing the uncertainty (i.e. numerical error estimation) issue in CFD simulations (e.g. Refs. [58–61]).

Moreover, concerned about the accuracy and reliability of CFD simulations, Blocken and Gualtieri [62] applied a ten-steps approach of disciplined model practice (set out by Ref. [63]) to CFD modelling of natural ventilation in a football stadium case study. The approach presented encompassed and extended the existing best practice guidelines for CFD model development by addressing particular questions that would enhance the decision-making process during CFD model development (e.g. purposes for modelling, modelling context, selection of model features, quantification of uncertainty). Furthermore, motivated by the lack of detailed case studies in which the CFD simulations were validated with on-site measurements, Blocken et al. [64] developed a general CFD simulation and decision framework for evaluating pedestrian wind comfort and safety in urban areas. The framework was based on existing best practice guidelines and applied to a complex real-life scenario. Next, the importance, scales, possibilities and limitations of CFD application in urban physics were also outlined [65], with ten tips and tricks presented towards accurate and reliable CFD simulations to complement existing CFD best practice guidelines with a focus on the outdoor and indoor urban environment. Those tips related to setting boundary conditions, carrying out grid convergence and validation studies and reporting results, among others. Some of the examples mentioned above relate to CFD modelling of urban environments, but they emphasise the importance of following systematic and disciplined methods to obtain credible results. Furthermore, good outdoor modelling is important for obtaining good prediction of the indoor environment through correctly specified boundary conditions.

3.1. CFD model development

The internal airflow in buildings is unique because of the space geometry (e.g. Refs. [66,67]), ventilation type (e.g. Refs. [41,68]), heat sources (e.g. Refs. [69,70]) and contaminant sources (e.g. Refs. [71,72]). Thus, in order to accurately investigate indoor conditions using robust (i.e. numerically stable) CFD models, careful consideration in mesh generation, boundary conditions specification, choice of turbulence models and discretisation scheme, and ability to estimate the results accuracy are of extreme importance. Fig. 3 show the main steps to developing an effective CFD model. Each step is further explained in detail.

There are a number of CFD software tools available to users, including open-source, with the most popular OpenFOAM [73], and commercial codes, e.g. Ansys Fluent [74], STAR-CCM + [75], PowerFlow [76], or PHOENICS [77].

Uncertainties in CFD simulations may arise at different stages of model development. Those uncertainties may occur from (i) simplifications and assumptions in the geometry of the flow domain and boundary conditions, e.g. inlets, outlets, heat and contaminant sources; or (ii) measurement accuracy, e.g. equipment (equipment data sheets) and experiment (due to data analysis) accuracy, that needs to be taken into account for boundary conditions and model validation. Significant consideration must be given to the choice of turbulence and radiation models, and simulation type for the particular type of a flow modelled.

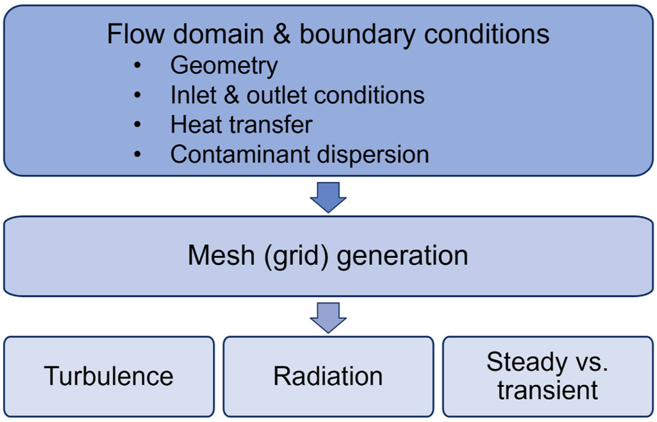

Fig. 3. Steps to the development of effective CFD models.

Furthermore, many types of errors may occur in a CFD simulation, including (i) discretisation errors (between exact and numerical solution), (ii) round off errors (due to the accuracy of a computer and the true value of a variable), (iii) iteration errors, (iv) physical modelling and (v) human errors. Thus, CFD models should be created using verified software, systematic grid refinement studies and trusted experimental data, that supports model validation, to ensure validity of the results. Furthermore, taking into account uncertainties/errors in the simulation and experimental data enables determination of the degree to which a model is an accurate representation of the real world.

The accuracy of CFD simulations strongly depends on model inputs specified by the modeller. The level of detail in the model, proper specification of inlet/outlet and wall conditions, as well as heat and contaminant sources are crucial, in order to develop credible and robust CFD models that represent indoor environments accurately. The correct specification of CFD boundary conditions influences not only the results accuracy, but also numerical stability of the model. Many suggestions and guidelines regarding this topic are available in technical documentation of CFD codes. A sensitivity analysis to identify the parameters at the boundaries that have a dominant effect on CFD predictions seems to be a useful strategy [9]. Furthermore, Djunaedy [78] proposed a guideline to select the appropriate simulation approach for certain flow problems. The guideline used sensitivity analysis to select the appropriate complexity and resolution of simulations, including the convective heat transfer coefficient as a parameter for the decision to use CFD.

There are CFD studies which provide accurate predictions of natural ventilation flows when the interior of the building is considered as the computational domain, and the ventilation flow rates are prescribed as boundary conditions at the window openings. However, from a design point of view, it is important to know if CFD can predict ventilation flow rates given initial and boundary conditions for temperature and far-field wind conditions, so that both indoor and outdoor environments must be modelled [9]. In these cases, the two environments are linked by an interface at the openings of the building, forming the wind pressure coefficient [79]. The recommended size of outdoor environment is application-dependent but there are highly cited references that provide widely used rules of thumb ([80,81]).

Before modelling a complex environment of a specific indoor space, starting with a simple geometry is a good practice. Simpler models can help better understand the principles of fluid flow and capabilities of CFD in the particular scenario, with a lower computational cost. Srebric et al. [82] showed that simplified human simulators can provide accurate temperature profiles within the modelled room. Furthermore, Topp et al. [83] explored the impact of human manikin's geometry on contaminant distribution and its personal exposure in a room with the displacement ventilation. The research did not find any significant difference between the simple rectangular shaped manikin and more complex humanlike geometry when predicting personal exposure. However, the contaminant concentration distributions around the manikin were different for two types of geometries due to different convective flows. When the interest is focused on the airflow around the human simulators, more care should be taken when specifying boundary conditions. Thus, more recently some research [84] highlighted the strong effect of computational thermal manikin simplifications on the thermal airflow field prediction, especially in the vicinity of manikin surfaces. A mesh decimating algorithm was used, which helped reduce computational cost keeping accurate predictive capabilities. Zukowska et al. [85] showed significant influence of thermal insulation and the design of clothing and chair, as well as the blocking effect of a table on the thermal plume above a sitting manikin.

In terms of inlet/outlet conditions specification, previous research [31] stressed the importance of an accurate estimation of the velocity profiles at the openings, as it is critical in proper calculation of airflow entering the building. Cao and Meyers [86] investigated the influence of turbulent inlet boundary conditions on airflow characteristics and pollutant dispersion in a mechanically ventilated enclosure, emphasising the importance of imposing realistic turbulent boundary conditions for turbulence models. Previous studies found the external ambient temperature to have larger effect on the temperature distribution in the buoyancy-driven naturally ventilated atrium than the thermal load inside the building [32]; while the stratum ventilation supply air temperature had a significant impact on thermal comfort of the occupants in an office [87]. Furthermore, Jansen et al. [88] carried out laboratory measurements to study the development of an air jet from a controlled natural ventilation grill for different outdoor conditions. Those measurements could define detailed boundary conditions for a CFD model to investigate indoor environmental conditions.

In the field of heat transfer modelling, Pan et al. [89] investigated thermal and sunlight performance of a highly glazed waiting hall of a train station. Validation with field measurements confirmed the ability of CFD to predict complex thermal phenomena in highly glazed spaces, as long as boundary conditions were properly specified. Furthermore, Gendelis and Jakovičs [90] found the location and type of the heater, air infiltration through the room's envelope and solar radiation sources having a big influence on the airflow inside the room. Park and Holland [91] studied the effect of convective heat source vertical location in a room with displacement ventilation. The heat source location was found to have a significant effect on the level of air temperature stratification and the behaviour of the gravity current inside the room. While, Rundle et al. [92] showed the superiority of discrete transfer radiation model above the Monte Carlo model to simulate radiation heat transfer in atria accurately, even with a coarse mesh.

Heat from the human body is transferred to the environment by convection, radiation, evaporation and respiration. Kilic and Sevilgen [93] showed that the most heat from the human body to the environment is released by radiation. Srebric et al. [82] and Loomans [94] recommended the convection to radiation (*C:R*) heat flux ratio for human simulators as 30:70 and 50:50, respectively. Moreover, Norton et al. [95] in their study of heat transfer from calves in a livestock building found that, unless the efforts involved in model development may be repaid by the results accuracy, the simulations should be kept as simple as possible (e.g. with an assumption of a fixed ratio between convective and radiative heat transfers from animals).

There have been many concerns about the air quality in built environments and negative effects of the contaminant dispersion on occupants' health and product quality, e.g. Refs. [96,97]. Thus, many studies have explored the topic of contaminant sources and distribution inside indoor spaces. Validated CFD simulations provided valuable information about the airborne contaminant source location and transport mechanisms in an aircraft cabin [98]. Srebric et al. [82] proposed to represent the indoor contaminant source by an area source in CFD model that is larger than the physical size of the contaminant source in the real environment, in order to increase the speed of the convergence process. This would not influence the accuracy when the source point is in a well predicted airflow field. However, caution must be taken when analysing the source point located in a complicated airflow field. Poussou et al. [99] utilised CFD simulation validated with the measurements in a small-scale water-based model in order to explore the influence of moving persons on the airflow and contaminant transport inside an aircraft cabin. Furthermore, Saidi et al. [71] showed that the contaminant source motion and its path influenced the contaminant dispersion inside a cleanroom to a great extent, and Nielsen [100] illustrated the influence of humidity on exhaled water-contained droplets which might have contained viruses or bacteria. As evidenced in the Covid-19 pandemic, improving indoor air quality requires urgent attention, particularly in naturally ventilated spaces. In that respect, previous studies utilised CFD to investigate the airborne pathogen transmission of Covid-19 in a generic confined space under different ventilation strategies, e.g. Ref. [101].

Mesh (or grid) generation is an important step in the development of a CFD model. A model domain needs to be divided into smaller and non-overlapping subdomains (cells) where the flow physics (i.e. discrete values of flow properties, such as pressure, velocity, temperature, etc.) are solved numerically [102]. There are two main types of mesh generation: structured and unstructured. For the structured meshes all mesh lines are regularly distributed. The unstructured meshes do not require the regularity condition and they consist of freely assembled cells (e.g. polyhedral cells). Due to their relative easiness in setting up the meshing conditions (and the algorithms to generate the mesh from that), the unstructured meshes are very popular in commercial CFD codes, even though they are more complicated to generate and more computationally expensive than the structured meshes.

Mesh quality is important in controlling simulation errors and, thus, should be given sufficient consideration. Significant measures of mesh quality include mesh orthogonality, expansion and aspect ratio. Bad quality cells are usually located in very narrow places, and thus, deleting them would not affect the results significantly [103]. This deleting process can be done by different utilities and is included in some meshing procedures, e.g. in OpenFOAM [104].

A successful mesh generation process is complex and often time consuming. However, most commercial CFD codes are equipped with user friendly interfaces that enable modellers to quickly develop adequate meshes in reasonable time frames.

Meshing strategies frequently used by research that addresses natural ventilation problems in buildings include the refinement in regions where large gradients are expected (e.g. boundary layers near walls and thermal sources), gradually increasing in size towards the domain's boundaries, and in some cases the use of adaptative mesh refinement in both thermal and dynamic boundary layers and high turbulence areas where high thermal or velocity gradients take place ([104,105]). High Reynolds numbers in wind engineering and natural ventilation applications, which demand integrating through the viscous sublayer, often require substantially fine grid resolutions in particular in the near-wall regions [106]. Generally, a conventional wisdom is to avoid placing cells in the buffer layer and place the nearest node to the wall in the viscous sublayer so that the dimensionless y + distance is around 1 which, with the general limitations on growth rate, will impose restrictions to the size of mesh elements near walls.

Furthermore, sometimes it is not the mesh itself, but the model used what has the more significant impact on simulation results [107]. Thus, in some cases, bad predictions of certain flow characteristics (such as reattachment) seem to be due to the use of certain RANS turbulence models and not to the mesh choice. On the other hand, models such as detached eddy simulation (DES), seem to suffer from possible grid induced separation where flow becomes separated through insufficient mesh refinement, leading to inaccurate results [108].

From a practitioner standpoint, the model and the grid resolution are closely coupled so that a very good model for a specific application will achieve satisfactory predictions only if the mesh resolution matches the specific model.

Choosing the appropriate turbulence model is crucial for creating a reliable and accurate CFD simulation. The performance of various turbulence models for simulating airflows in built environments has been published widely in previous literature. A comprehensive study by Zhang et al. [109] evaluated, in terms of accuracy and computational cost, the performance of eight turbulence models (RANS, LES and DES) to simulate indoor airflow. The accuracy of those models was evaluated by comparison with experimental data available in literature. The results revealed that generally LES provided more detailed flow features than RANS, but with much higher computational cost and not always higher accuracy. Overall, the performance of turbulence models depended on the flow characteristics. Based on that study, Fig. 4 summarises tested turbulence models that proved good and acceptable accuracy for various airflow types.

Fig. 4 has limitations, where only LES represents the scale-resolving methods and it does not detail the type of wall modelling used with the LES (e.g. wall modelled LES, wall-adapting local eddy-viscosity, standard wall functions, etc.). Some guidelines on scale-resolving simulations are available in Refs. [110,111]. There are also hybrid approaches (e.g. delayed DES, improved DES, extra LES [112]) which offer a plethora of options, along with the generalized k-ω model that has the flexibility to be tuned for natural flows [113]. However, many new developments of hybrid models are all solely within commercial codes, e.g. Ansys [114], and thus open access CFD codes do not have these newer advanced models.

This section outlines some previous research studies that investigated different turbulence models suitable for natural ventilation.

With respect to buoyancy driven flows, Liu et al. [32] searched for the most accurate turbulence model, in order to simulate indoor air temperatures in an atrium building with a buoyancy-driven ventilation, where knowledge of temperature stratification was required. It was observed that the RNG *k-ε* and zero-equation turbulent schemes provided good agreement with the measurements in the heated zone; while for the buoyancy-driven conditions of an atrium space, the laminar and zero-equation CFD models were most accurate. Furthermore, a systematic validation of the CFD model of an atrium with on-site measurements noted that the *k-ω* turbulence model accurately simulated indoor fluid flows and heat transfer [92]. Hussain et al. [115] also evaluated the performance of various turbulence models (one-equation, standard *k-ε*, RNG *k-ε*, realisable *k-ε*, standard *k-ω* and shear stress transport (SST) *k-ω*) to simulate indoor conditions in atria. The results of CFD simulations, including discrete transfer radiation model, were compared to the measurements in two existing buildings. Relatively good agreement was found between measured data and all turbulence models' results. However, the SST *k-ω* turbulence model proved to be the more suitable than *k-ε* models for modelling atria spaces.

The study of Ray et al. [116], which used a full-scale naturally ventilated atrium to validate three CFD turbulence models (RNG k–ε, k–ε, and LES), showed that all of them were able to predict experimental temperatures with a root mean square error below 1.2 K. Other research [117] highlighted the ability of k-ω models to reproduce temperature distribution accurately, while k–ε models failed in doing so. The work emphasised the importance of the iterative convergence criteria on the results in terms of temperature and age of air. In a recent work, Chen et al. [9] used unsteady RANS (URANS) to couple outdoor and indoor environment and predict the time evolution of the temperature field in the atrium. The objective of this work was to address this gap in full-scale model validation of buoyancy-driven natural ventilation in atrium buildings.

The investigation of turbulence modelling (standard *k-ε*, the RNG *k-ε*, SST *k-ω* and laminar model) in CFD simulations of office spaces were provided in a comprehensive study by Stamou and Katsiris [118]. Calculations displayed the ability of all tested models to predict the main qualitative features of the flow and temperature stratification well. However, from the quantitative point of view, the SST *k-ω* model demonstrated the best agreement with measurements. Srebric et al. [82] investigated different turbulence models (L-VEL, standard *k-ε,* RNG *k-ε*) on the example of an office room with human simulators and displacement ventilation. It was recommended to use one of the *k-ε* models, as they were found to predict airflow and heat transfer in that scenario very well. Moreover, Karimipanah et al. [119] investigated indoor conditions inside a classroom with confluent jet ventilation system. The predictions of air temperatures and velocities for two CFD models (with standard *k-ε* and RNG *k-ε* turbulence models) were compared with the measurements in a full-scale setup classroom with manikins. The air temperature prediction was acceptable for both turbulence models. However, the RNG *k-ε* model was found to predict air velocities in an occupied zone much

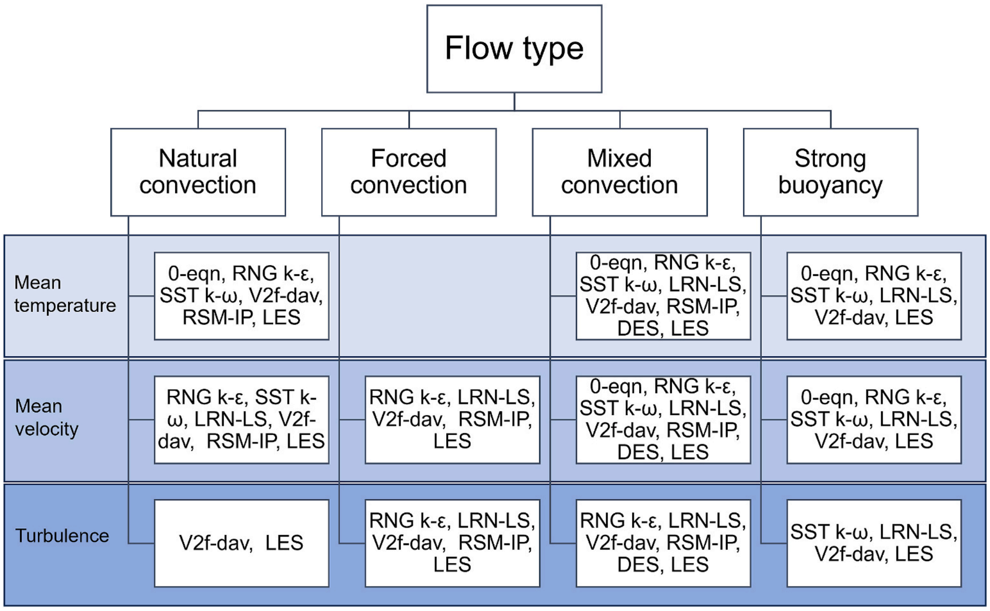

Fig. 4. The best suited turbulence models for various airflow types, based on [109].

better than the standard k-ε model. A study by Ruponen and Tinker [120] evaluated methods for estimating thermal comfort indoors. The work used validated CFD results to test k-ε and SST k-ω turbulence models for modelling thermal and isothermal indoor airflows. The k-ε model showed better agreement with measured data in isothermal case. However, in non-isothermal scenario the SST k-ω performed better. Other examples of applying various turbulence models to simulate airflow and temperature distribution inside mechanically ventilated spaces include [121,122].

In terms of large internal environments, Shen et al. [123] estimated the ventilation rates in naturally ventilated livestock building under varied wind conditions. The research investigated several RANS turbulence models (k-ε, RNG k-ε, realisable k-ε, k-ω and SST k-ω) and compared to wind tunnel measurements. The overall ventilation rate through the building was best predicted by standard k–ω turbulence model.

LES has been established in the wind industry, e.g. Refs. [124,125]. However, there are published studies that utilise LES for indoor simulations, e.g. Refs. [126,127]. While LES can provide more accurate and reliable results than RANS, it also requires more simulation complexity and thus higher computational resources [128].

In general, the selection of the turbulence model has influence on the prediction of airflow characteristics. Some studies of cross-ventilation in buildings concluded that RANS models were not able to predict the distribution of the turbulent kinetic energy because they failed to capture the features in transient flow (including Kelvin-Helmholtz instabilities and jet flapping) on the resolved airflow pattern [129]. Ventilation rates, which depend both on the turbulence model and the calculation method (opening velocity method or tracer gas decay method), seem to be more satisfactorily predicted by LES than by RANS models in wind-driven ventilation problems [44], due to its ability to capture wind flow fluctuations, although LES requires significantly more computation time (5–60 times). On the other hand, although boundary layer separation and reattachment length have a significant impact on pressure distribution and, consequently, on building ventilation, they are sometimes difficult to estimate accurately even if advanced models such as LES are used [107].

Modelling radiation usually must be included when simulating airflow in a building; specifically when significant heat sources are present, there is a large difference between room surface temperatures (due to building orientation, glazing), and when the space is ventilated by pure buoyancy. Some research reported relative differences in air temperature gradients that ranged between 60 % and 80 % when radiation heat transfer was and was not modelled [130].

Radiation can be modelled using different algorithms that generally solve the radiation transport equation, obtain the source term for the energy equation and the radiative heat flux at walls [74]. Due to the dependence on spatial coordinates, local direction coordinates and frequency, the formal solution of the equation is time-consuming, and approximations are used for directional and spectral dependencies. Table 1 summarises some of the most commonly used radiation models and their main characteristics. There are guidelines to select an appropriate model for certain problems, which are generally based on the optical thickness (which represents the ability of a given path length of gas to attenuate radiation of a given wavelength) of the flow domain as a discriminating parameter, model capability of taking different features into account: scattering and wall emissivity, particle effects, or reflection on walls [74].

From the literature review on CFD modelling of atrium and office buildings, it can be seen that surface to surface and discrete transfer radiation models are the most commonly used. In some other studies, radiation is not considered or modelled in a simplified manner by measuring temperatures at walls or by setting combined heat transfer coefficients. On the other hand, in more complex configurations, like highly glazed buildings, attention must be paid to sun patch modelling, the internal distribution of shortwave and longwave radiation within the building, direct retransmission, reflection to the outside, etc. [131]. Radiative heat transfer and, specifically, convection to radiative heat flux ratio are critical for the accurate estimation of temperature profiles around human simulators in indoor environments [82].

Table 1
Description of the most common radiation models and main characteristics [74].

Model	Main assumptions	Advantages	Limitations
P-1 model	-Directional dependence is integrated out in radiative transfer equation.	-Little computational cost. -Scattering is included. -It performs well when optical thickness is large (greater than 3).	-All surfaces are diffuse. -Gray radiation. -Loss of accuracy, depending of geometry complexity, if optical thickness is small. -Radiative fluxes from localized sources or sinks are overpredicted.
Roseland model	-Similar to P-1, although the intensity is the black-body intensity at the gas temperature.	-Faster than P1 model. -It allows anisotropic scattering.	-Only used for optically thick media (greater than 3).
Discrete ordinate (DO) model	-One radiative heat transfer equation is solved for every discrete number of solid angles or beam directions.	-Conservative method: it leads to balance even for coarse discretisation. -Comprehensive: It accounts for scattering, semi-transparent media, specular surfaces and wavelength-dependent transmission.	-Intensive computational cost in problems with large number of beam directions (ordinates). -Do not perform ray tracing.
Discrete transfer radiation model (DTRM)	-Radiation leaving the surface element in a certain range of solid angles are approximated by a single ray. -Refractive index is assumed to be unity.	-Predict radiative transfer between surfaces without explicit view factor calculations. -Wide range of optical thickness.	-All surfaces are diffuse. -Scattering is not included. -Gray radiation. -Computationally very expensive when there are too many surfaces to trace rays and many volumes crossed by the rays. - Accuracy limited by the number of rays and mesh.
Surface to surface (S2S) model	-Energy exchange between two surfaces depend on their size, distance and orientation. Absorption, emission or scattering are ignored. Surfaces are gray and diffuse.	-Good for modelling the enclosure radiative transfer without participating media. -Faster than discrete ordinate and discrete transfer radiation model per iteration.	-All surfaces are diffuse. -Gray radiation. -It cannot be used for participating media problems or periodic boundary conditions. -Computational cost increases rapidly when the number of surface faces increases.

Numerous practical engineering flows, as well as the flows occurring naturally, are turbulent, three dimensional and unsteady. The RANS approach uses turbulence models to model the scales of instantaneous turbulent motion. Steady state simulations using RANS have become the industry standard [132], primarily due to their affordability in terms of computational expense. The limitations of steady state simulations have been increasingly highlighted in recent years, with advances in computational ability placing high performance computing within reach of numerous businesses and research institutions. When the knowledge about the transient behaviour of the flow is necessary, the RANS approach is not sufficient. Furthermore, the URANS was attempted to solve a transient flow, but failed to account for unsteadiness [133].

LES does not adopt the conventional time-averaging RANS approach with additional transport equations being solved. Large scale motions of turbulent flow are computed directly in LES, with only small sub-grid scale motions being modelled. LES is more accurate than RANS and URANS approaches, since the large eddies contain most of the turbulent energy. Durrani et al. [134] evaluated LES and URANS in CFD modelling of multiple steady states in natural ventilation. Both LES and URANS solutions captured the existence of three steady states observed in controlled experiments. LES was proven to be more accurate in predicting the temperatures inside the enclosure compared to URANS; 0.15 % discrepancy for the LES, and a 3-fold larger discrepancy for the URANS. However, the drawback of using LES was its expense.

When predicting internal flows and natural ventilation in the built environment, RANS can be used with high accuracy e.g. Ref. [29]. However, Blocken [65] warned of oscillatory convergence in steady RANS simulations that might occur when inherently transient flows are forced into a steady simulation. This may imply that a single converged solution will not be obtained, and the solution will depend on the number of preceding iterations.

In conclusion, and although recent hybrid strategies have been investigated [135], LES has been found to be more successful than RANS in predicting qualitative and quantitative flow phenomena for natural ventilation, at the cost of greater computational and time expense [134]. While RANS is currently the most commonly used approach, all indications point towards an expanding future use of LES and unsteady simulations in the built environment, since they seem to be more capable of explaining the variability found in indoor environments.

3.2. *Verification*

The first step in the process of estimating credibility and accuracy of CFD models is verification. Verification determines if the CFD simulation accurately predicts the conceptual model, as shown in Fig. 5. Verification does not prove whether there is any relationship between the simulation results and the real world [8]. There are two types of CFD verification: (i) CFD code verification and (ii) CFD model verification. The first one (i) involves error evaluation from a known solution to find incorrect implementations of conceptual models and input errors in the code.

Previous research [1,136] presented examples of code verification by evaluating the performance of commercial (PHOENICS, Fluent, CFX) and academic codes (Clima 3D) against the experimental data for typical ventilation case studies. The work concluded that, although the agreement was better for velocities than temperatures, which was attributed to the use of different methods for modelling heat transfer rather than the code itself, the commercial codes represented a powerful tool for the simulation of different building environments. Other research [137] concluded that the selection of CFD codes for a study depends on the complexity and characteristic of the model, desired turbulence model for a study, and ease of use for the graphic user interface.

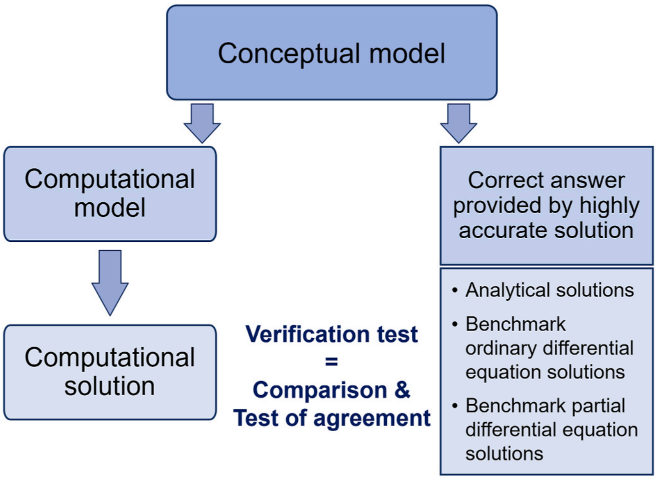

Fig. 5. Model verification schematic, redrawn from Ref. [8].

The second type of CFD verification (ii) focuses on error estimation to define the accuracy of CFD calculation and finding the error band of the model results [138]. The accuracy of CFD simulation depends on the discretisation errors and, thus, on the number of cells used in a mesh. A model with a larger number of mesh cells provides a more accurate solution; however, this is at the price of higher computation cost and calculation time [102].

Despite the development of modern computing power, it is still quite expensive to obtain a grid independent solution for the natural ventilation problems ([139,140]). Although there is sometimes a potential use of reduced-scale models to save computational resources [141], increasing the number and refinement of meshes are imperative to get reliable and accurate computational results. But this is not always attainable due to limitations of computational time and cost. In some cases, finer meshes might not improve the accuracy anymore, and coarser meshes might still give accurate results [104].

Hence, CFD model verification is an important step to find the appropriate compromise between the level of uncertainty and computational requirements. As shown previously [56], comparing predictions directly to measurements without performing a grid refinement (also called sensitivity or independence) study could give the modeller a false sense of confidence in the CFD results. CFD model verification can be done in a qualitative and quantitative manner. A qualitative verification involves graphical comparison between the simulation results for different mesh densities. A quantitative verification requires a comparison between the "quantities" of the results and may utilise comparison methods, such as relative difference, mean squared error, etc. Moreover, in order to unify reporting of the CFD model verification through the grid refinement studies, the grid convergence index (GCI) was developed [142]. It has been shown that systematic grid refinement studies, to establish a grid independent solution, are straightforward and reliable technique for numerical uncertainty quantification [58]. Hence, the GCI has become a widely used parameter to perform model verification studies in the CFD community, e.g. Refs. [59,143].

Table 2 presents different validated CFD studies of built environments published as journal articles since year 2000. This table contains research relating to both natural and mechanical ventilation and indicates whether the qualitative and quantitative grid verification and validation studies were reported. Despite the specific guidelines regarding the estimation of discretisation errors through grid sensitivity studies [143], grid verification has not always been reported in the literature when presenting the results of CFD models of built environments. About a half (47 %) of the studies shown in Table 2 included the results of grid verification, and amongst those grid verification studies 69 % were quantitative. What is more, only three studies, in a group of ninety studies presented in Table 2, performed model verification using the GCI method [143] to estimate the model uncertainty due to discretisation errors.

3.3. *Validation*

The second step on the road to credible CFD models is validation. CFD model validation determines how accurately the model represents phenomena in the real world, as shown in Fig. 6 [8]. This is done through the qualitative and/or quantitative comparison between the CFD results and quality assured experimental data (measured with reliable and calibrated equipment, with experimental error considered). It can be difficult to estimate the results accuracy for complex CFD

Table 2
Grid verification and model validation studies in CFD models of built environments, updated from Ref. [11].

Indoor space type	Publication	Grid verification reported		Model validation reported	
		Qualitative (graphically)	Quantitative	Qualitative (graphically)	Quantitative
Agricultural building	[144]	no	no	yes	Comparison & Relative difference [%]
	[145]	no	no	yes	Comparison & Difference & Relative difference
	[95]	no	Coefficient of variation of root mean square deviation	yes	Comparison & Coefficient of variation of root mean square deviation
	[146]	no	no	yes	no
	[147]	no	no	no	Difference & Relative difference [%] & Normalised mean squared error
	[104]	yes	Mean relative error bounded & comprehensive error (magnitude and phase error [148])	yes	Mean relative error bounded & comprehensive error (magnitude and phase error [148])
	[149]	no	Absolute differences(°C and m/s)	yes	Correlation & Difference
Atrium space	[39]	yes	Relative difference [%]	yes	no
	[150]	no	no	yes	Comparison
	[32]	no	Root mean square error	yes	Correlation & Difference
	[151]	no	no	yes	Relative difference [%]
	[92]	no	no	yes	Difference & Relative difference [%]
	[152]	no	no	yes	Comparison & Relative difference [%]
	[115]	yes	Comparison & Relative difference [%]	yes	Comparison & Relative difference [%]
	[153]	yes	Comparison	yes	Comparison & Relative difference [%]
	[116]	no	no	yes	Comparison & deviation
	[9]	no	Absolute differences [°C]	yes	Root mean square error [°C]
Car park	[154]	no	no	yes	no
	[155]	yes	no	yes	Comparison
	[156]	no	no	yes	no
	[157]	yes	no	yes	no
Classroom	[119]	no	no	no	Comparison
	[158]	no	no	yes	no
	[159]	no	Absolute differences (Pa, m/s, °C)	yes	Relative difference [%]
Cleanroom	[160]	no	no	yes	no
	[161]	no	no	yes	Relative difference [%]
	[162]	no	no	yes	no
Data centre	[163]	no	no	yes	no
	[164]	no	no	yes	no
	[165]	no	no	yes	no
	[166]	yes	Absolute differences (°C)	yes	Root mean square error (°C)
Hospital room	[67]	no	no	no	Relative difference [%]
	[167]	no	no	yes	no
	[72]	no	no	yes	no
	[168]	no	no	yes	no
Ice skating arena	[169]	no	no	yes	no
Industrial factory	[170]	no	no	yes	no
	[171]	no	no	yes	Deviation
	[172]	no	no	yes	no
	[140]	yes	Normalised root mean square error	yes	Relative difference [%]
	[173]	yes	GCI	yes	no
Model building	[174]	no	Relative difference [%]	yes	Relative difference [%]
	[175]	no	no	yes	Comparison
	[35]	no	no	yes	Relative difference [%]
	[36]	no	Relative difference [%]	yes	no
	[176]	no	no	yes	Comparison & Relative difference [%]
	[177]	no	Comparison	yes	Comparison & Coefficient of variation of root mean square deviation
	[29]	no	Relative difference [%]	yes	Comparison & difference [%]
	[178]	no	Relative difference [%]	yes	Comparison & Regression analysis
	[179]	yes	Relative difference [%]	yes	Comparison
	[180]	yes	Relative difference [%]	yes	Relative difference [%]
	[44]	yes	GCI	yes	Four validation metrics: hit rate (q), fractional bias (FB), factor of 2 of the observation (FAC2),
Model room	[46]	no	no	yes	Comparison
	[181]	no	no	yes	Comparison & Relative difference [%]
	[1]	no	no	yes	Difference & Relative difference
	[66]	yes	no	yes	no
	[182]	no	no	yes	no
	[183]	no	no	no	Comparison & Relative difference [%]
	[184]	yes	Relative difference [%]	yes	Comparison
	[185]	no	no	yes	Relative difference [%]
	[186]	no	Relative difference [%]	yes	no
	[187]	no	no	yes	Comparison
	[188]	yes	no	yes	Difference
	[189]	no	no	yes	Relative difference & Euclidean difference
	[190]	no	no	yes	Comparison
	[40]	yes	no	yes	Relative difference [%]

(*continued on next page*)

Table 2 (*continued*)

Indoor space type	Publication	Grid verification reported		Model validation reported	
		Qualitative (graphically)	Quantitative	Qualitative (graphically)	Quantitative
	[191]	no	Comparison & Relative difference [%]	yes	no
	[192]	no	no	no	Comparison & Difference
	[193]	no	no	yes	no
	[194]	yes	no	yes	no
	[70]	no	no	yes	Comparison
	[195]	yes	Relative difference [%]	no	Relative difference [%]
	[196]	yes	no	yes	Relative difference [%]
	[197]	yes	no	yes	Root mean square error [°C]
Office	[118]	no	no	yes	Comparison & Difference
	[82]	yes	no	yes	no
	[198]	no	no	yes	no
	[199]	no	no	yes	no
	[200]	no	no	yes	Difference
	[201]	yes	no	yes	Relative difference [%]
	[202]	yes	Deviation	yes	Comparison & Relative difference [%]
	[28]	yes	GCI	yes	Comparison & Difference
	[203]	yes	no	yes	Relative difference [%]
	[101]	yes	no	yes	Deviation
Operating theatre	[204]	no	no	no	Comparison
	[205]	yes	no	yes	no
Stadium	[206,207]	no	Normalised relative difference [%]	yes	Deviation
Train station	[208]	no	no	yes	no
	[209]	no	Relative difference [%]	yes	Difference

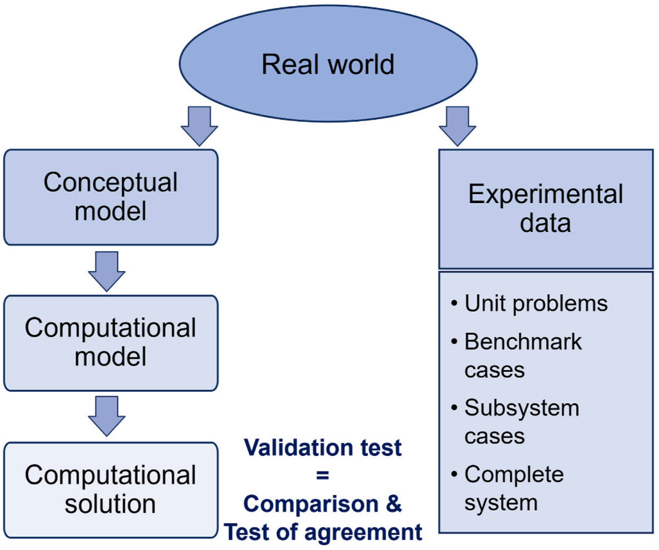

Fig. 6. Model validation schematic, redrawn from Ref. [8].

studies. Hence, verification and validation studies, together with uncertainty analysis, should accompany any reliable CFD simulation [62].

Often, a CFD validation procedure involves only qualitative, graphical comparison of model results and experimental data [210]. Moreover, it is common in CFD studies that only the general conclusion, about 'acceptable', 'satisfactory', 'good', etc. prediction, is drawn when comparing numerical and experimental results. However, the specification and application of validation criteria (also called metrics by some works) is the most important practice in validation activities [211]. Those criteria are used to quantitatively compare simulation and experimental results. Validation criteria should quantify errors and uncertainties in both simulated and experimental data. Literature indicates that some attempts to quantify the differences between the simulation and measurements have been made. For instance, a previous study [212] developed validation metrics that should apply to physical systems in fluid dynamics, heat transfer and solid mechanics. The proposed metrics were based on the statistical concept of confidence intervals to validate computational models with experimental data. Ierardi and Barnett [213] tested linear regression and relative error as validation methods on examples including fire plume and ceiling jet CFD modelling. A study by Audouin et al. [189] quantitatively compared CFD results of a room fire simulation with full-scale experimental measurements. The comparisons were made using a relative difference method and a normalised Euclidean distance method. Furthermore, the percent error method was used to quantitatively assess the differences between the CFD model results and the measurements (i) in a small-scale naturally ventilated building [152], or (ii) in a full-scale building with a single-sided natural ventilation system [176].

There are several methods to obtain validation data for computational models: (i) analytical models, (ii) small-scale experimental models, (iii) full-scale experimental models and (iv) field measurements. The analytical models have been sparsely reported in literature [6]; even though, those models are probably the most mature amongst the methods for predicting ventilation performance in buildings and are still quite effective and powerful [183]. Small-scale experimental setups are cheaper and easier to build than the full-scale models. However, when using small-scale setups scaling issues associated with the thermo-fluid dimensionless parameters may occur [6]. Field measurements provide reliable information about the conditions in the real environment. Even though, they may be expensive, time consuming and limited by the amount of instrumentation available and obstacles in the operating buildings, field measurements are used to provide the boundary conditions for the computational model and/or validate simulation results. However, field data are always to some degree uncertain, and this uncertainty can only marginally be caused by the instrumentation error [214]. The variability and unexpected changes of conditions in normally operating (especially naturally ventilated) buildings are challenging when collecting and interpreting measured data to support numerical simulations.

Table 2 (Section 3.2) demonstrates that 33 % of reviewed validated CFD studies of indoor environments (naturally and mechanically ventilated) were only qualitative. Moreover, a review of published literature found the lack of specific criteria for validating CFD simulations of built environments. Table 3 gives a more detailed overview of the validated CFD studies of naturally ventilated indoor spaces, considering the validation data source and type. 37 % of the presented CFD studies validated their results with field measurements, 20 %

Table 3
Overview of validated CFD studies of naturally ventilated built environments, updated from Ref. [11].

Indoor space type	Publication	CFD code	Validation data source	Ventilation type	Validation data type			
					Air temp.	Air velocity	Flow rate	Other
Agricultural building	[95]	STAR-CCM+	Small-scale model & field measurements	Natural	✓	✓		Heat flux
	[147]	Fluent v6.2	Field measurements	Natural	✓			
	[104]	OpenFOAM	Small-scale model & field measurements	Natural		✓		
	[149]	Star CCM+	Full-scale setup	Natural	✓			
Atrium space	[39]	CFX v4.4	Analytical model & small-scale model	Natural			✓	Buoyancy force (reduced gravity) & Interface height (stratification level)
	[150]	Fluent v6.2	Full-scale setup	Natural & Mechanical	✓	✓	✓	Wall temperature
	[32]	AirPak v2.1	Small-scale model	Natural	✓			
	[152]	Phoenics v3.5	Small-scale model	Natural	✓	✓	✓	
	[153]	Fluent v6.3.26	Field measurements	Natural (Hybrid solar assisted)	✓			
	[116]	Fluent	Field measurements	Natural	✓	✓		Airflow visualization
	[9]	Fluent v2021 R1	Field measurements	Natural	✓			
Car park	[156]	FDS	Field measurements	Natural & Mechanical				Propane concentration
	[157]	Fluent R16	Full-scale setup	Natural				Helium concentration
Model building	[174]	–	Small-scale model	Natural		✓		Mean pressure coefficient
	[35]	AirPak	Field measurements	Natural				Mean age of air
	[36]	Ansys CFX 12.0	Small-scale model	Natural		✓		
	[176]	Fluent v6.2	Field measurements	Natural	✓	✓	✓	Turbulence intensity
	[177]	Ansys Fluent v12.0	Small-scale model	Natural			✓	Pressure coefficient
	[29]	Fluent v6.3	Small-scale model	Natural		✓		
	[178]	StarCCM +6.06	Small-scale model	Natural				Air exchange rates & age air
	[179]	Fluent v6.3	Small-scale model	Natural		✓		
	[180]	Fluent 2015	Field measurements	Natural & Mechanical	✓			
	[44]	Fluent v19.2	Small-scale model	Natural		✓		
Model room	[46]	–	Full-scale setup	Natural	✓	✓		Air change rate & Turbulence energy spectra
	[183]	Fluent v5.5	Network model	Natural			✓	
	[40]	Fluent v6.2	Field measurements	Natural		✓		
	[191]	Phoenics 2009	Small-scale model	Natural		✓		
	[192]	Fluent v6.0	Full-scale setup	Natural	✓	✓		Relative humidity
	[194]	Fluent v6.3	Small-scale model	Natural		✓		
	[195]	Fluent v6.3	Full-scale setup	Natural	✓			
	[28]	Ansys CFX v12.1	Field measurements	Natural	✓	✓		
	[203]	Fluent v17.0	Small-scale model and full-scale set-up	Natural & Mechanical	✓	✓		
	[101]	Fluent v19.0	Small-scale model	Natural		✓		
Stadium	[206,207]	Fluent v6.3	Field measurements	Natural		✓		Wind direction

utilised measurements in full-scale setups and 43 % in small-scale setups. This shows that the small-scale set-ups together with the field measurements have been the most popular data sources to validate CFD models. Air velocity was the most popular validation parameter (used in 57 % of considered studies) followed by air temperature (used in 46 % of considered studies).

3.4. Calibration

Calibration has been described as the process of adjusting physical or numerical parameters in a CFD model to improve the agreement between model results and experimental data [8]. Once the computational model is calibrated with quality assured experimental data, new model scenarios can be simulated and their results can be accepted with a low level of uncertainty [215]. However, the CFD model calibration process is not straightforward. As CFD simulations can be very sensitive to many user-defined computational parameters (such as boundary and initial conditions, convergence limits, etc.) detailed sensitivity studies are necessary to evaluate the impact of those parameters on model results. Once the most influential input parameters are known, they can be tuned and the calibration process may be finalised.

Previous research extensively investigated the influence of various CFD model input parameters on simulation results in the field of built environments. For instance, validated CFD results supplied valuable findings about the influence of internal partitioning on ventilation performance in rooms [66], or proved the great influence of obstructions on indoor airflow patterns [181].

In terms of mechanical ventilation, Chen et al. [193] explored the effect of input parameters (such as jet discharge height, diffuser geometry, supply airflow rate and confinement from surrounding environment) on airflow features in a room with an impinging jet concept ventilation strategy. Moreover, validated CFD models gave an indication of the significant influence of a thermal plume generated above human occupant, on the particle transport in rooms with displacement ventilation [70]. A recent study [216] performed a sensitivity analysis to investigate the impact of turbulence models and inlet boundary conditions on CFD modelling of non-isothermal mechanical ventilation in a generic enclosure.

From the natural ventilation point of view, Horan and Finn [30] studied the impact of external wind speeds and directions on ventilation rates inside the atrium space. To support the calibration process, van Hooff and Blocken [207] utilised coupled urban and indoor wind flow CFD simulations to assess the influence of wind direction and urban surroundings on ventilation rates in a semi enclosed stadium. The effects of window opening's width on the airflow inside a room [217] or openings' configurations on the airflow in a model room [34] have been previously investigated. In addition, Gao and Lee [35] researched the influence of openings' configurations on ventilation performance in residential units.

Hajdukiewicz et al. [28] developed a formal calibration methodology for CFD models of naturally ventilated indoor environments, which explained how to quantitatively and qualitatively verify, validate and calibrate CFD models. The validation workflow required validation criteria to be specified based on the objectives of the CFD simulation of indoor environment (e.g. office spaces require thermal comfort of the occupants, while data centres or cleanrooms demand rigorous indoor conditions). The proposed calibration methodology included parametric analysis utilising the response surface technique to support a robust calibration process.

The CFD calibration works described above mainly focused on how to find the optimal input parameters to achieve a calibrated model. However, Jiang et al. [218] developed a method to calibrate the results of a CFD simulation, based on sparse sensor observations in an air-conditioned room. The research found that the performance of this method closely related to the number of sensor observations and the sensing locations.

4. Discussion and conclusions

Table 4 summarises the main and most common guidelines and recommendations derived from this extensive literature review and that a researcher or user may consider in each step of the CFD simulation/modelling of a natural ventilation problem in a built environment. Within these important steps (selection of a domain and boundary conditions, meshing process, turbulence model, etc.) the one related to solution convergence and residual analysis has been shown explicitly here to highlight its links with other relevant stages of CFD modelling and for the sake of simplicity. Also, useful references have been included to provide more information about each specific issue.

This narrative review demonstrates the capabilities of, and the challenges posed by CFD models in analysing indoor environmental conditions in buildings, with particular attention given to natural ventilation flows. The work summarises published literature to present a wide range of CFD studies of those environments, emphasising the fact that knowledge and experience are necessary to create reliable CFD simulations.

Since analysing natural ventilation requires interpretation of highly variable boundary conditions, the study shows the importance of quality assured experimental data to support the credibility of CFD simulations. Furthermore, methods, that utilise parametric analysis to guarantee the quality of the input boundary conditions that most influence the simulation results, are particularly critical when dealing with natural ventilation flows.

The review points to the existing best practice guidelines that explain in detail how to verify, validate and estimate uncertainty in CFD simulations. However, this review has found that a significant number of reviewed studies (relating to validated CFD simulations of indoor environments shown in Table 2) did not report grid verification (53 %) or performed only qualitative validation of results (33 %) without clearly specified validation criteria.

Moreover, the study identified a lack of specific criteria for validating CFD models of naturally ventilated environments, with different

Table 4
Summary of the most common guidelines and conclusions drawn from literature review related to CFD modelling of indoor built environments (*those shown in italics are specific to natural ventilation*).

Step	Guidelines and recommendations	Useful references
Flow domain and boundary conditions	-Progress from simple to more detailed geometry of scaled or full-scale models. -Use sensitivity analysis to identify boundaries with dominant effect on flow characteristics. *-At a building design stage, it can be interesting to model both indoor and outdoor environment,* e.g. *considering no wind condition, different wind angles and wind pressure coefficients.*	- Best practices: [219]. - Dimensions of outdoor flow domain: [80,81].
Mesh	-Apply mesh refinement in regions of interest (boundary layers at walls, thermal sources, turbulent regions, etc.). -When solving the viscous sublayer, place the nearest node to the wall so that the dimensionless distance is around 1. -Check mesh quality and mesh-turbulence model dependence.	[102,104,219,220]
Turbulence model	-Performance of turbulence models generally depends on flow characteristics, as shown in Fig. 4. -Use simple approaches (e.g. indoor zero-equation model) to provide good initial fields for more advanced turbulence models. -In general, in non-isothermal scenario the SST k-ω performs better than other RANS models. *-LES and URANS can be good options to couple outdoor and indoor environments.*	See Fig. 4 for references.
Radiation model	-Modelling radiation is critical in buildings with important heat sources, large difference between room surface temperatures, airflow driven by buoyancy, etc. -Surface to surface model is the most common approach. -In case of no-radiation, the temperature or convective heat flux must be specified.	Ansys Fluent [74].
Steady/transient simulations	*-RANS can usually predict internal flows and natural ventilation with high accuracy.* -Check the presence of oscillatory convergence in (steady) RANS simulations. In these cases, URANS or hybrid models can be suitable alternatives. -LES seems to explain the variability found in indoor environments better but it is still computationally more expensive than RANS.	RANS, URANS, LES: [132,133].
Convergence/ residuals	-In a well-posed problem, the residuals (usually RMS) of all variables must show a monotonic convergence. -Flow patterns must show a sensible behaviour. -In general, targets for residuals of mass, velocity components and turbulence measures (10^{-5}-10^{-3}) are greater than for energy residuals (10^{-6}-10^{-5}). -Check if mass flow and energy imbalances are small enough (0.01%–1%) before considering the solution is converged.	Extracted from the works listed in Table 3.

(*continued on next page*)

Table 4 (*continued*)

Step	Guidelines and recommendations	Useful references
	-Check monitoring points is a good practice. -Use relaxation factors to help convergence.	
Verification	-Two types of verification: CFD code verification and CFD model verification. The current commercial (and open source) codes are verified, so the focus should be on model verification. -It is good practice to use a systematic grid refinement (e.g. GCI) study for numerical uncertainty quantification.	-Code verification: [1,136]. -Model verification: [58,142,143].
Calibration/ validation	-Sensitivity studies should be considered to assess the impact of different parameters (boundary/ initial conditions, etc.) on model results. -There are different methods to obtain validation data. -Compare numerical and experimental results quantitatively: use of validation metrics.	-Calibration: [28]. -Validation: [62, 104].

experimental data sources utilised in studies ranging from small- and full-scale setups to field measurements. Air velocity and temperature where the most popular validation parameters for CFD model development of naturally ventilated built environments.

The research shows the value of explicit and documented methodologies for validating and calibrating CFD simulations to develop quality assured and flexible (for which new scenarios for the calibrated model can be simulated and their results can be accepted with a low level of uncertainty) models that accurately represent environmental conditions in naturally ventilated buildings. The study reviews literature to systematically guide and explain the process of CFD model development, including the assessment of simulated data and field measurements when developing calibrated CFD models of naturally ventilated built environments.

For the first time, this work provides an extensive overview of verification and validation studies relating to CFD models of different built environments (included in Table 2), and detailed validation studies of naturally ventilated spaces (included in Table 3). Furthermore, the review summarises the most common guidelines and conclusions drawn from literature relating to CFD modelling of naturally ventilated built environments (included in Table 4) and, thus, makes contribution to researchers who are commencing work in this field. The review summarises the state-of-the-art and presents an outlook on individual components related to the CFD methodology. With that the research serves both the reader that is looking for supporting information to perform a CFD analysis of a natural ventilation flow problem, and a reader that is interested in a generic improvement of CFD for this type of application.

Natural ventilation systems in buildings are being increasingly adopted to both reduce building energy demand through passive cooling, and provide good indoor environmental quality for occupants, with adaptive comfort theory in mind to the contemporary insights towards adaptive thermal comfort theory. This results in reduced need for mechanical ventilation and relaxed conditions for thermal control in buildings. Thus, developing credible CFD models of naturally ventilated built environments will contribute towards better design and operation of buildings that meet the requirements of a sustainable built environment.

The review identifies a scope for further research on newer turbulence models, such as those developed by commercial codes, that have the potential to improve accuracy and simulation cost and could be applied to the built environment. The arrival of Lattice Boltzmann simulations on the scene, after being applied and validated extensively in automotive and aerospace applications, could be suitable for built environment applications, e.g. Refs. [76,221]. Other LES-only solvers on the cloud and graphics processing unit solvers are also being investigated, promising detailed LES simulations at lower costs. Finally, newer meshing technologies developed by commercial codes, e.g. Refs. [75, 219], are allowing for very complex geometry to be realised within simulations, so fewer geometrical simplifications are needed.

CRediT authorship contribution statement

Magdalena Hajdukiewicz: Methodology, Writing – original draft. **Francisco Javier González Gallero:** Writing – review & editing. **Paul Mannion:** Writing – review & editing. **Marcel G.L.C. Loomans:** Writing – review & editing, Supervision. **Marcus M. Keane:** Conceptualization, Writing – review & editing.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interestsMagdalena Hajdukiewicz reports financial support was provided by European Commission. Francisco Javier Gonzalez Gallero reports financial support was provided by University of Cadiz. Magdalena Hajdukiewicz reports financial support was provided by Higher Education Authority.

Data availability

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