Indoor microbial growth prediction using coupled computational fluid dynamics and microbial growth models

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Abstract

This study investigates, using in-situ and numerical simulation experiments, airflow and hygrothermal distribution in a mechanically ventilated academic research facility with known cases of microbial proliferations. Microclimate parameters were obtained from in-situ experiments and used as boundary conditions and validation of the numerical experiments with a commercial CFD analysis tool using the standard k–ε model. The findings revealed good agreements with less than 10% deviations between the measured and simulated results. Subsequent upon successful validation, the model was used to investigate hygrothermal and airflow profile within the shelves holding stored components in the facility. The predicted in-shelf hygrothermal profile were superimposed on mould growth limiting curve earlier documented in the literature. Results revealed the growth of *xerophilic* species in most parts of the shelves. The mould growth prediction correlates with the microbial investigation in the case studied room reported by the authors elsewhere. Satisfactory prediction of mould growth in the room successfully proved that the CFD simulation can be used to investigate the conditions that lead to microbial growth in an indoor environment.

Keywords

Hygrothermal performance; in-situ experiments; microbial growth prediction; CFD simulation; indoor microclimate.

1 Introduction

With increased universal concern on urbanisation, rising energy cost, depletion of fossil fuels and greenhouse gas emission, the need for building energy efficiency remains a great concern to government and private agencies globally. The building sector becomes more of concern as its energy usage stands at about 40% of the global utilisation and contributing up to nearly 40-50% of the world carbon emissions [1, 2]. The bulk of this consumption goes for heating and cooling operations with values of over 60% [3, 4]. Building HVAC systems are tasked with the provision of adequate thermal comfort as well as removal of contaminants and other indoor pollutants [5, 6]. As a consequent, an inadequate indoor ventilation will not only results in making occupants thermally uncomfortable but also making the building unhealthy.

Unhealthy buildings lead to Sick Building Syndrome (SBS) and other Building Related Illnesses (BRI). Similarly, poor ventilation is detrimental to building fabrics and indoor stored components of archives in the museums, library and other mission critical indoor environments. In health care facilities, the ventilation system is tasked with preventing cross infection risks while maintaining adequate thermal comfort to both the patients, the caregivers and visitors. On the contrary, despite the high energy consumption, the HVAC contributes to making building unhealthy [7]. Also, evidence exists of an association between building energy efficiency improvements, elevated moisture level and microbial infestation with other deteriorative occurrences [8, 9]. Therefore, there is a need to consider the hygrothermal performance of building when implementing energy efficiency and/or conservation measures. The built environment, over the past few decades, has therefore witnessed the emergence of building performance diagnostics. Building performance assessments are executed on the existing buildings in retrofit upgrades as well as new ones even before they are built. According to Chen [10], building performance appraisal are executed by: analytical and empirical methods, numerical simulation and experimental measurements. While the experimental approach is found most significant as it generates validation data for analytical and numerical simulation models, field experiments are expensive in terms of cost and access to free houses [11].

The rapid improvement in computer power in the past two to three decades has significantly influenced the development and progress of computational models fluid dynamics research [12]. As reiterated by the authors, there is a change in speed from about 10^9 Flops in 1984 to 10^{13} Flops in 2002, evidence that is corroborated by the observation of Li and Nielsen [13]. Various computational tools have therefore been developed as reviewed by Woloszyn and Rode [14] and Delgado, et al. [15]. These tools are grouped into building energy simulation (BES), heat air and moisture (HAM) and computational fluid dynamics (CFD) models with each of them having their strengths and weaknesses. Hence, the performance assessment can be accomplished with a single tool or by coupling several tools for improvement in their prediction of both energy performance, moisture performance and indoor environment quality analysis [12, 16]. According to Allard, et al. [12], the coupling between building performance tools can be done within a single program suite or by external data exchange between varying tools. A good overview can be found in the body of literature [17, 18].

Despite these advancements, numerous uncertainties exist in building performance assessments. With good uncertainty clarifications, interpretation of results can be correctly done thereby increasing the reliability of obtained results. Experimental errors or uncertainties can arise from the set-up, data collection and measuring equipment [5]. Detailed of a statistical approach for assessing instrumentation uncertainty in field experiment is presented by the author [19]. Similarly, numerical experiments include error sources as modelling simplifications, mathematical and numerical models, and boundary conditions [12, 20]. Standard procedures for the execution and reporting of numerical experiments have evolved to reduce such uncertainties [21, 22]. Ascertaining uncertainty from the simulation codes, the guidelines recommend benchmarking selected code with a previously documented numerical and experimental solution. In addition, the guidelines recommend correlating simulated results with the measured values to ensuring that the results obtained from simulation are less prone to errors. For errors and uncertainties due to the computational grid, grid dependency analysis remains the industry standards for improving discretisation accuracy.

Moulds are pervasive in nature as they are primary decomposer of organic materials from plants and animal remains. As a result of mould ubiquity, they are omnipresent in an indoor environment as microbiologically clean buildings do not exist [23]. Despite their ecological importance, mould may be harmful to not only the indoor stored collections but also the occupants' health [18]. Mould limiting growth factors are numerous ranging from spores, sufficient temperature, nutrients and moisture. Mould does not require light to grow [24] and as such believe in light as a growth factor appears erroneous. In predicting mould occurrence, a good indicator of growth had been found to be moisture related as according to British Standard Institution [25], the occurrence of mould species are indicative of excessive moisture. Therefore, a holistic approach is needed to predict where, when and under what conditions mould grows [16] as early detection is often difficult until growth has advanced. There are various models for mould growth prediction although no widely accepted evaluation method exists [26]. Vereecken and Roels [27] reviewed mould prediction models . The prediction models adopt the presence of moisture either in liquid or vapour form by the humid air attaining a value above certain threshold limits.

From the foregoing, it is evident that the sustainability needs require energy efficient ventilation systems that are found with detrimental effects on the buildings and its users. Building performance diagnostic tools have developed over the past decades with the advancement in computational power and assessment metrics. Microbial proliferations in indoor environment possess a danger to occupants' health as well as the building and its stored components, hence early prediction becomes necessary. This study, therefore, presents the results of mould growth prediction in a mechanically ventilated academic research facility with known cases of microbial proliferations using in-situ experiment and computational fluid dynamics (CFD) simulation coupled with mould prediction model.

2 Materials and methods

2.1 In-Situ experiments

2.1.1 Experimental setup

The case-studied room measures 5.2 m long by 4.8 m wide and 3.0 m high. It is air-conditioned and ventilated by a constant air volume (CAV) air handling unit (AHU) that controls the airflow, thermal and hygric distribution in the room. The air distribution is a mixing ventilation type with a ceiling-mounted four-way square supply diffuser (600 mm x 600 mm) and a rectangular extract grille (600 mm x 300 mm). The lighting system consists of six numbers ceiling-mounted fluorescent fittings (600 mm x 1200 mm) with two numbers 36W lamps. The air outlets, as well as light fittings, were flushed with the ceiling surface. The furniture comprises of metal shelves to keep stored components. Figure 1 shows the layout and measurement positions in the in-situ experimental setup.

Figure 1 – Layout and measurement positions in the in-situ experimental setup

2.1.2 Instrumentation and measurement

The in-situ experiments, which involved microclimate investigations, were in two manifolds: steady-state and time-series. The steady state experiment involves collection of data that include (1) room surface temperature from wall, floor and ceiling (with Testo infra-red thermometer); (2) room ambient air temperature, relative humidity and speed (with ALNOR AVM440 anemometers); and (3) supply and exhaust temperature, relative humidity and air flow rate (with ALNOR AVM440 anemometers). In the time-series measurement, data loggers (EL-USB-2-LCD+) were mounted at the room centre, supply and exhaust outlets. Data from the steady state measurements were use as input boundary conditions for the CFD simulations while those from time-series measurement employed in the model validation.

2.2 Numerical simulation

2.2.1 Governing equation

In the numerical simulations, incompressible steady state Navier-Stokes equation coupled with the standard k–ε turbulence model were employed. Equation (1) shows the general form of the Navier-Stokes equation [12, 28]. Table 1 presents the dependent variables (ϕ), effective diffusion coefficients (Γϕ), and the source term (Sϕ) for each of the flow parameters in equation (1).

$$\frac{\partial}{\partial t}(\rho \varphi) + div\left(\rho V \varphi - \Gamma_{\varphi} grad \varphi\right) = S_{\varphi} \quad (1)$$

Where ρ is the density, V is the velocity vector, ϕ is the dependent variable in the flow field to which the equation applies (temperature, velocity, pressure, etc.), Γϕ is the turbulent diffusion coefficient and Sϕ is the source or sink term of the variable ϕ.

Table 1 The dependent variables (ϕ), effective diffusion coefficients (Γϕ), and the source term (SΦ) for each of the flow parameters

Equation	Φ	Γ_Φ	S_Φ
Continuity	1	0	0
x momentum	u	μ	$-\partial P/\partial x$
y momentum (vertical)	v	μ	$-\partial P/\partial y$ - ρg
z momentum	w	μ	$-\partial P/\partial z$
Enthalpy	$C_p T$	λ	Q
Concentration	c/ρ	d	Q_m
k equation	k	μ/σ_k	$G - \rho\, \varepsilon$
ε equation	ε	μ/σ_ε	$C_1\, \varepsilon\, G/k - C_2\, \rho\, \varepsilon_2/k$
$\mu = \mu_{lam} + \mu_t$ $\mu_t = \rho\, C\mu\, k^2/\varepsilon$ $G = \mu[2[(\partial u/\partial x)^2 + (\partial v/\partial y)^2 + (\partial w/\partial z)^2] + (\partial u/\partial y + \partial v/\partial x)^2 + (\partial v/\partial z + \partial w/\partial y)^2 + (\partial u/\partial z + \partial w/\partial x)^2]$ C1 = 1.44, C2 = 1.92, Cμ = 0.09, $\sigma_H = 0.9$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$			

2.2.2 Benchmark case

It is essential for users of a specific CFD tool to carry out benchmark case by reproducing an existing study with reported experimental and numerical data [5]. Such benchmark assessment ascertains the ability of the CFD tool to replicate the experiment. Also, such benchmark experiment verifies users' ability of the CFD code. As a result and owing to the documented procedures [21, 22, 29], the present study carried out a benchmark case from Spitler [30] experiments. The benchmark is aimed at: (1) ascertaining the capability of the selected CFD code to simulate and reproduce the selected physical phenomena as previously documented with minimal deviations, and (2) to equip the researcher with necessary experience in making informed judgment from simulation results. The original study measures and compares temperature, airflow and other parameters along the room height, exhaust outlet and indoor ambient. Basic input parameters in the benchmark case are – Room size: 4.57m x 2.74m x 2.74m high; air supply and exhaust outlets: size = 903.7mm x 400mm, temperature = 21 °C, airflow rates = 15ACH; heated panels on all wall surfaces with temperature = 30 °C.

2.2.3 Experimental model setup

3D modelling (Figure 2) of the experimental room was created in the CFD analysis tool. The walls, floor and ceiling were modelled as adiabatic since the room is bounded by other rooms with similar air conditions. In the model, the shelves were placed nearly 25 mm from the wall surfaces and sat directly on the floor. The stored items were modelled as a row of objects rather than individual items to conserve computational resources. Equally, since the objects allow air movement between them, they were modelled as resistances (porous object) with 20% openings. The simplification is considered sufficient to represent the airflow through the objects as similarly adopted by Fletcher, et al. [31]. One of the many benefits of CFD simulation is the ability to place virtual data loggers at different points of interests other than the in-situ measurement positions. The virtual data loggers allow assessment of the hygrothermal conditions

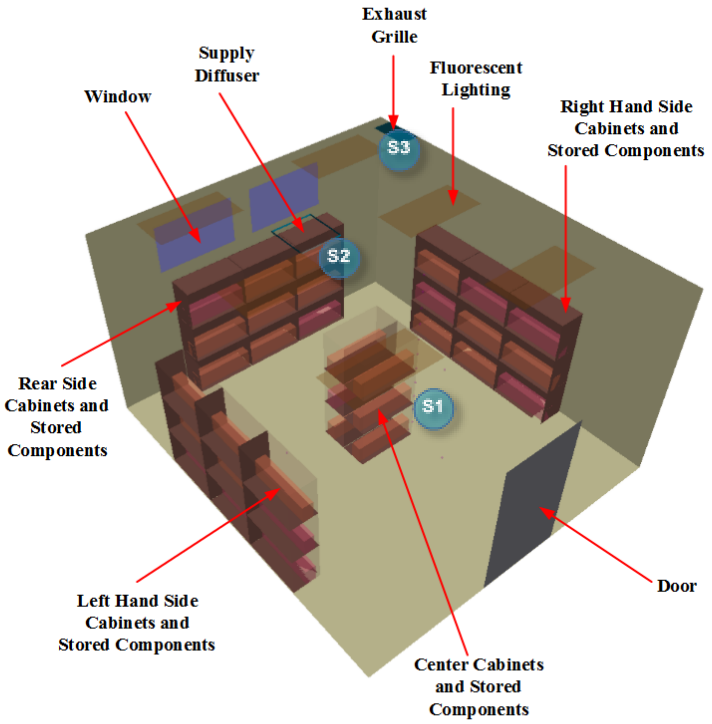

Figure 2 – Space Layouts with positions of supply, exhaust and other components of the case study room. S1, S2 and S3 are virtual data loggers' positions

within the shelves and stored items that seems difficult to achieve on the site. Figure-1 shows details of the space layouts with positions of supply, exhaust and other components of the case studied room.

2.2.4 Boundary condition, discretisation and grid dependency analysis

The source terms in equation 1 are provided as boundary conditions from the air outlets – supply diffuser (temperature = 15.5 °C, humidity ratio = 9.8 x 10^{-3} kg/kg, airflow rates = 0.61 m^3/s) and return grille (airflow rates = 0.61 m^3/s). Others are enclosures surface temperatures – walls (17.4 °C, 16.8 °C, 18.4 °C and 19.6 °C), floor (18.4 °C) and ceiling (17.3 °C) and lighting heat gains (6 x 72 W). The return grille humidity ratio as well temperature are to be computed by the CFD simulation. As the accuracy of CFD results depends on the grids' quality [12, 21], the entire simulation domain was discretised using structured grid approach. Grid refinement was performed around the supply and return outlets to cater for high gradients often associated with air terminal devices thereby improving the prediction of velocity flow field [1]. The baseline grid was of coarse type with a total 4752 cells. Grids fine-tuning was executed with a total of 9885 and 39935 for medium and fine grids respectively. In this study, grid dependency analysis was carried out with virtual measurement of the hygrothermal parameters on a vertical section at centre of the modelled room. Series of simulations were executed using coarse, medium and fine grids.

2.2.5 Model validation

Subsequent to the satisfactory grid selection, the model validation is executed between the measured and simulated thermo-hygric parameters in the room centre. In the validation, the study adopted percentage root-mean-square deviation (PRMSD) approach [4, 32]. PRMSD is obtained as a single value for the reference points as evaluated from Equation (2):

$$PRMSD = \sqrt{\left(\frac{\sum_0^n \left(\frac{C_m - C_s}{C_m} \times 100\right)^2}{n}\right)} \tag{2}$$

Where: C_m is the measured parameter; C_s is the simulated parameters and n is the number of points under considerations.

2.2.6 Simulation of hygrothermal profile on stored items and mould growth prediction

Extended simulations were carried out on the model in which key parameters were selected for further analysis to predict the hygrothermal parameters (T and RH) within the shelves and racks. In addition, points along the x-axis were selected to assess the indoor indoor thermohygric distributions at planes before (0.75 m) and after (2.25 m) the supply diffuser. Results of the predicted hygrothermal profiles were superimposed on the mould growth isopleth of Clarke [33, 34]. A similar approach had been previously reported in the work of Clarke [16] where building performance simulation code (ESP-r) was used to predict the hygrothermal conditions leading to growth in a mould infested house.

3 Results and discussions

3.1 Benchmark case

Figure 3 shows the airflow contour plots measured at plane cutting across the centre of the supply outlet. The airflow contour plots revealed similar flow pattern between the CFD simulated (Figure 3b) and the Spitler experiment (Figure 3a). The cold air drops from the supply outlet and flows parallel to the floor until it gets to the opposite wall. Subsequently, the air rises along the wall and when it gets to ceiling level, the air vortexes out. Overall, the airflow contour reveals a very good agreement between simulated and Spitler results. Results of the percentage root-mean-square deviation (PRMSD) between CFD simulation and the experimental thermal data of Spitler revealed a maximum value of 7%. This deviation falls within the documented acceptable limits [1, 32, 35, 36]. The results, therefore, indicate that both the CFD simulation code and the investigator were able to produce a good agreement with a previously documented experimental data.

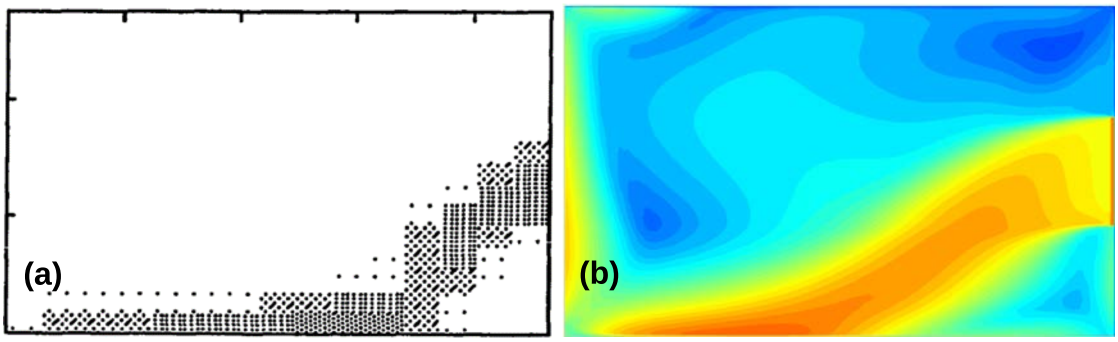

Figure 3 – Benchmark case: airflow profile with side mounted supply
(a) Spitler [30] experimental airflow pattern (b) CFD simulation airflow pattern

3.2 Grid dependency analysis

Figure 4 shows the results of grid dependency assessments. The prediction from the coarse grid was far low in comparison to medium and fine grids. Nevertheless, for most of the measured cases, the fine mesh under-predicts the basic flow parameters as compared to medium grids. This reason, coupled with longer computational time resulted in selecting the medium grid for further analysis.

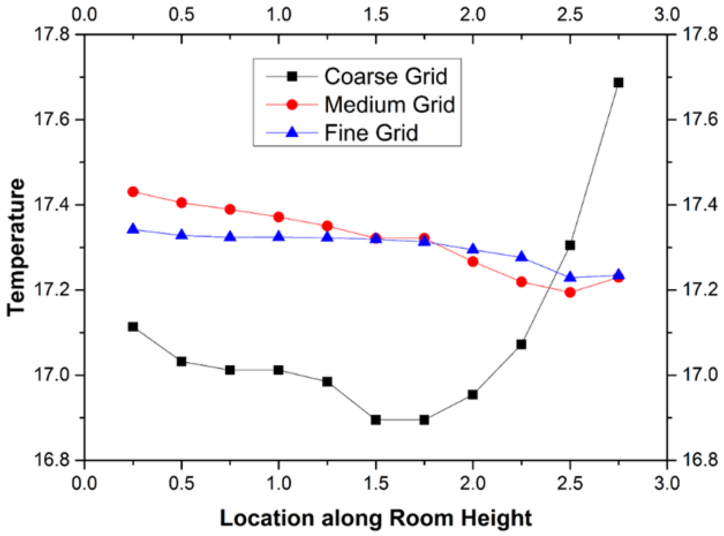

Figure 4 – Grid dependency analysis

3.3 Validation of simulation and measured data

PMRSD between the measured and simulated parameters for the in-situ as well as simulated experiments gave 2.6% and 4.1% respectively for T and RH. The validation results performed better than earlier studies that acceptable deviations between the measured and simulated values in the numerical investigation should be in the range of 5% [35] and 10% [1]. In the study of [36], the difference was found to be higher than 5-10% where their experiment reported a deviation of more than 25%. A value of 6.7% deviation was reported in the work of [32].

3.4 Thermal and hygric profile

The mean thermal and hygric performance in the occupied zone were found as T = 17.2 °C and RH = 78.4%. Figures 5 and 6 show the thermohygric profiles at x = 0.75m and 2.25m respectively. The upper part close to ceiling shows high temperature and low humidity due to heat emission from lighting while concentrated cold region is shown on the air-stream around the supply diffuser (Figures 5a and 6a).

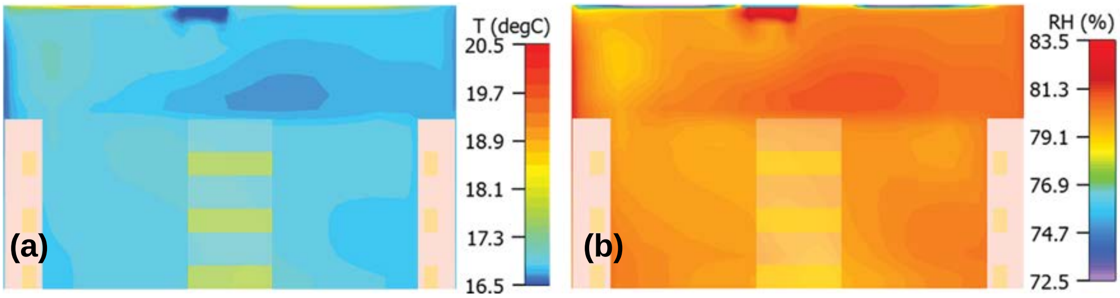

Figure 5 – Thermohygric profile at *x* = 0.75m (a) T contour (b) RH contour

Also, regions close to the shelves were found with low thermal and elevated hygric gradients (Figures 5b and 6b). Overall, the entire room revealed thermal and hygric stratifications not only within the room but also around the shelves. These suggest that the air in the room is not well distributed. The consequence of such stratification in thermal and high hygric profiles could result in microbial proliferation as reported in a similar study elsewhere [37].

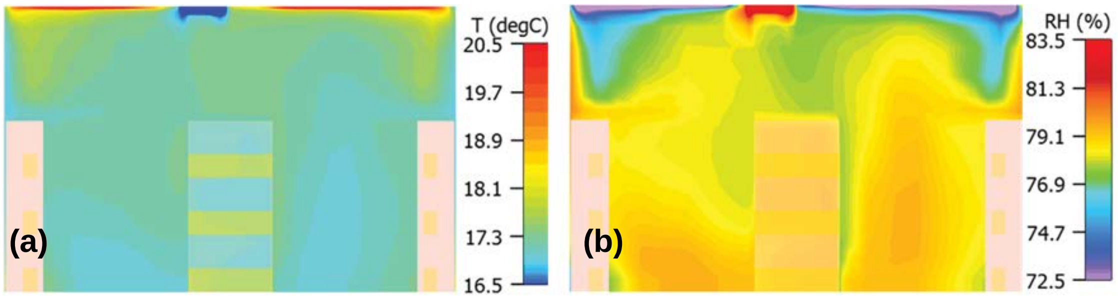

Figure 6 – Thermohygric profile at *x* = 2.25m (a) T contour (b) RH contour

3.5 Mould growth prediction

The predicted in-shelves hygrothermal conditions were superimposed on the mould growth isopleths. Figure 7 shows the predicted mould growth in the case-studied room. Each of the marked points represents stacks within the respective shelves. In most cases, the predicted mould groups were between categories A to C – the xerophilic (dry-loving) species of mould classifications [16, 33, 34]. Results of mould predictions were in agreement with that of microbial sampling protocol reported elsewhere [38]. It found that the viable mould species in the room were mainly *Penicillium sp.* and *Aspergillus sp.* These identified species were categorised as xerophilic (dry-loving) in the documented research of Clarke [33, 34].

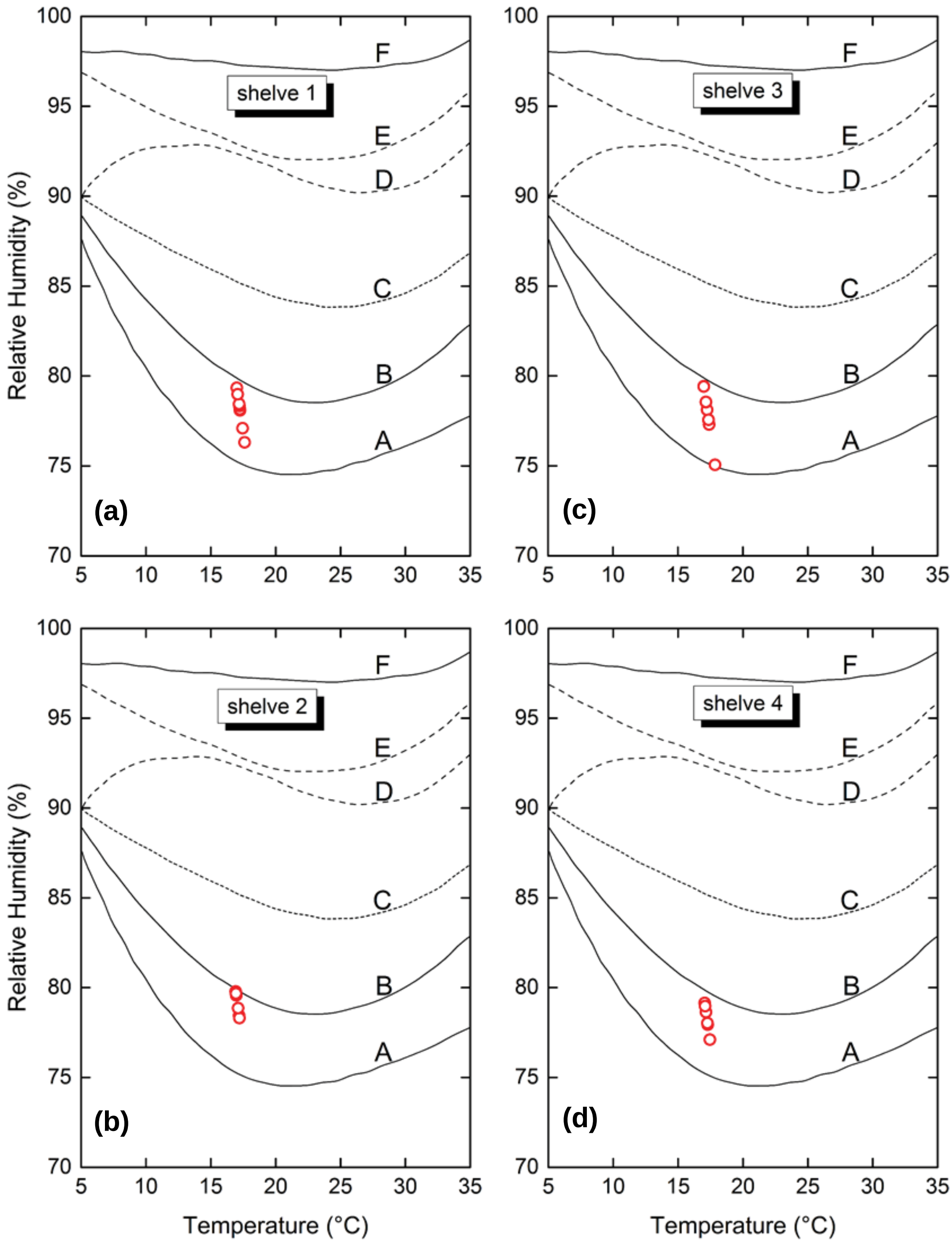

Figure 7 – Mould Growth Prediction on Stored Components in: (a) shelve #1 (b) shelve #2 (c) shelve #3 and (d) shelve # 4

4 Conclusions

The study combines in-situ and numerical experiment with mould growth model to predict mould growth in a case studied building. Benchmark studies in CFD simulation improves reliability on the analysis tool in its application of the governing equations. Similarly, validation of the simulated results with measured data provides certainty about the model implementation as well as the adopted procedures for the case consideration. Results of benchmark studies revealed a similarity between the documented and presently simulated results. The findings indicate that both the CFD analysis tool and the researcher are capable of providing solutions for indoor airflow performance assessments. The good agreement achieved between the in-situ and numerical experiments in the present study with less than 10% deviation ascertains the model's capability in representing the case-studied room. Most parts of the room revealed thermal and hygric stratifications thereby suggesting the not well-distributed air in the room, a situation that is consequential to microbial proliferations.

The results of mould growth prediction were found in correlation with the microbial investigation in the case studied room. Xerophilic mould – *Penicillium sp.* and *Aspergillus sp.* were found in the case-studied room. Satisfactory prediction of mould growth in the room successfully proved that the CFD simulation can be used to investigate the conditions that lead to microbial growth in an indoor environment. It is a common practice in reality to optimise the design by running additional simulations. In the optimised simulation, various parameters can be varied and effects examined on the hygrothermal profile and mould growth likelihood. Such optimisation studies are beyond the scope of the present study and are therefore recommended for further future investigations.

5 Acknowledgements

The authors wish to acknowledge the assistance of Dr Niza Samsuddin, Dr Hairul Aini Hamzah as well as the Dean of Kulliyyah (Faculty) of Medicine IIUM together with the management and staffs of Daya Bersih during the studies.

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