# A NOVEL POST-PROCESSING CONTAMINANT TRANSPORT AND DECAY MODEL FOR ENERGYPLUS

Jonathon Taylor[1], Phillip Biddulph[2], Hector Altamirano[1], Clive Shrubsole[1], Payel Das[1], Anna Mavrogianni[1], and Mike Davies[1]
[1]The Bartlett School of Graduate Studies, UCL, London, UK
[2]UCL Energy Institute, UCL, London, UK

## ABSTRACT

This paper introduces PolyPol, a post-processing tool that calculates the transport and deposition of an unlimited number of contaminants from airflow data output from EnergyPlus simulations. In addition, the model is able to use data on temperature and humidity-related airborne pathogen decay or chemical reaction rates to estimate the loss or gain of species over time. An initial intermodel validation between the EnergyPlus Generic Contaminant Model, CONTAM, and PolyPol is performed, and the importance of dynamic indoor temperatures and water vapour concentration demonstrated. PolyPol is then used to model influenza levels in a pre and post-energy efficient retrofit terraced dwelling, accounting for building thermal, moisture, and ventilative behaviour, and biological decay.

## INTRODUCTION

Indoor Air Quality (IAQ) modelling is an important tool for understanding the exposure of building occupants to indoor air pollution. Pollutants can be classified as being chemical or biological contaminants. Chemical pollutants can include those from indoor sources, such as $NO_2$ from cooking and environmental tobacco smoke, and those from outdoor sources that are able to infiltrate into the dwelling, for example $PM_{2.5}$. Biological pollutants are also produced by indoor sources (for example, bioaerosols such as mould spores or pathogens released by infected building occupants), or from outdoor sources (infiltration of pollen or outdoor mould spores into the indoor environment).

There are number of tools available for airflow and IAQ modelling, including simple single-zoned models, multi-zonal models such as CONTAM (Walton G.N. & Dols, 2008) and the EnergyPlus Generic Contaminant Model (GCM) (US-DOE, 2013), or more complex Computational Fluid Dynamics (CFD) models. In multi-zonal airflow models, zones within buildings are treated as a series of nodes connected by airflow elements such as doors, cracks, and ducts.

The temperature and moisture content of air can affect airflow and therefore contaminant transport. Under typical conditions, buildings will experience dynamic zonal air temperatures depending on the thermal performance of the building and the behaviour of the building occupants. Equation 1 describes pressure losses across an airflow path.

$$\Delta P = (P_1 - P_2) - \left( \frac{\rho_1 v_1^2}{2} - \frac{\rho_2 v_2^2}{2} \right) + g(\rho_1 z_1 - \rho_2 z_2) \tag{1}$$

where $\Delta P$ is the pressure difference across the airflow path (Pa), $P_1$ and $P_2$ are the absolute pressures on either side of the airflow path (Pa), $\rho$ is the density of air (kg/m$^3$), $v_1$ and $v_2$ are the entry and exit velocities of the air (m/s), $g$ is the acceleration due to gravity (9.8m/s$^2$), and $z$ is the elevation (m). The first term refers to static pressure differences, the second term differences caused by wind speeds, and the third term differences due to air density. At low wind speeds, the third term becomes more significant. The density of air is typically calculated using the dry air and water vapour components of the air, and temperature (Equation 2).

$$\rho = \frac{P_d}{R_d T} + \frac{P_v}{R_v T} \tag{2}$$

where $P_d$ and $P_v$ represent the pressure (Pa) of the dry air component and water vapour, respectively, $R_d$ and $R_v$ represent the specific gas constant for dry air and water vapour (J/kg/K), and $T$ is temperature (K). Therefore, temperature and the water content of the air can influence airflow under low windspeed conditions.

**Indoor Contaminants**

Indoor air contaminant concentrations are typically modelled based on the addition of contaminants to a zone (from indoor sources, transported in contaminated air from other zones or outdoors, desorption, or produced through a chemical reaction), while contaminants are removed through chemical reactions, adsorption to building materials, filtration, biological decay and deposition. In addition to airflow, the temperature and water vapour of the indoor environment can influence the removal of contaminants in the air by affecting the survival or persistence of airborne biological contaminants, the rate of chemical reaction, the deposition behaviour of different pollutants, or the penetration of pollutants into the building. The interaction between air temperature, water content and indoor contaminant concentrations can vary according to the type of contaminant, examples of which include:

***Biological decay of microorganisms.*** Transmission of infectious microorganisms can occur through direct transmission (whereby an infected individual sneezes or coughs large droplets directly onto another person); airborne transmission (an individual inhales infected small particle aerosols); or direct contact (an individual comes in physical contact with an infected surface). The relative contribution of the different pathways to influenza transmission is not well understood (Brankston et al, 2007), although airborne transmission is increasingly thought to be an important contributor (Cowling et al, 2013).

The survival of microorganisms transmitted through the airborne pathway is thought to be related to indoor temperature and water content. Temperature is considered to be an important factor in the survival of airborne viruses, with viruses generally showing a greater persistence as temperatures decrease (Tang, 2009). The survival and transmission of aerosolised respiratory viruses have been correlated to indoor temperature and humidity (Hersoug, 2005; Chan et al., 1999), thereby increasing the risk of person-to-person transmission. The persistence of influenza in the indoor air has been found to be significantly correlated with absolute humidity levels (Shaman & Kohn, 2009).

The survival of airborne bacteria has also been observed to be related to the temperature and humidity of the air, although there is a much greater variation in how bacteria respond when compared to viruses (Tang, 2009). There is no clear pattern visible according to the structural characteristics of the bacteria and the temperature and water content-dependent airborne survival, and so survival is often considered at a species-level.

***Chemical reaction and emission.*** The concentration of chemical pollutants in the indoor air may also be influenced by indoor air conditions. The kinetic reaction rates of chemical contaminants in indoor air can be dependent on the air temperature (Nazaroff & Cass, 1986). Temperature and RH may also affect the emission rates of Volatile Organic Compounds (VOCs) from building materials (Xiong & Zhang, 2010).

***Penetration rate and deposition***. A number of studies have observed a relationship between relative humidity and the deposition velocity of indoor air pollutants, including $NO_2$ and $SO_2$ (Grøntoft & Raychaudhuri, 2004). The penetration factor of outdoor particles into buildings is dependent on particle size, and crack geometry and roughness (Chen & Zhao, 2011). This value can vary according to the ventilation, approaching one when windows are opened. Deposition rates have also been observed to increase when windows are closed, likely due to decreased indoor air turbulence reducing the likelihood of surface deposition (Long et al, 2001).

## Aims and Objectives

There are a number of modelling tools available that can be used to predict indoor air quality (IAQ), including the above-mentioned CONTAM and EnergyPlus. CONTAM is a tool developed by the National Institute of Standards and Technology (NIST) specifically designed for IAQ and ventilation analysis. EnergyPlus is a dynamic thermal simulation tool, capable of modelling airflow and contaminant levels using the Airflow Network and Generic Contaminant Model (GCM). One limitation of CONTAM is that it is not a dynamic thermal simulation program. Internal temperatures must be estimated, or imported from the results of dynamic thermal models such as EnergyPlus or temperatures measured in the field. In addition, CONTAM is not able to directly account for the hygrothermal properties of the building envelope, which can influence the internal temperature and water vapour concentration. Finally, the results of previous studies have demonstrated how coupled overheating and air pollution models can provide insight into how building properties and temperature-dependent occupant behaviour may affect indoor pollution levels (Mavrogianni et al, 2013); this relationship is in need of further investigation.

The introduction of the GCM into EnergyPlus v7.2 allows for the simulation of contaminant transport through modelled dwellings using a fully coupled dynamic thermal simulation model. In addition, the heat and moisture transport (HAMT) modelling capabilities of EnergyPlus mean that water content of the indoor air under operational conditions may be estimated, accounting for the moisture transport and buffering properties of the building envelope. However, EnergyPlus is currently limited to being able to simulate only a single contaminant, and neither EnergyPlus nor CONTAM can account for the influence of indoor air conditions on the decay, chemical reaction, deposition, and penetration of contaminants.

Therefore, a novel model (PolyPol) has been developed that allows multiple contaminants to be simulated at once using outputs from EnergyPlus, with temperature and humidity-dependent reaction and decay of the contaminating species accounted for. This paper outlines the initial development and testing of PolyPol and demonstrates how indoor temperature and water vapour concentration can influence contaminant levels. PolyPol is then used to estimate how the air-tightening of a terraced dwelling representative of the most common type of housing in London may influence the levels of viable airborne influenza inside a bedroom at night.

## SIMULATIONS

### Model Development

The PolyPol post-processing tool was developed in Python Version 3.3.2, and can account for the sum of contaminant loads from internal sources, removal through sinks, transfer due to interzone mixing, supply system airflow, infiltration and ventilation of outdoor air, and through diffusion between interior surfaces and zone air. Contaminant transport in PolyPol is governed by the movement of air, calculated by the EnergyPlus Airflow Network.

PolyPol operates in conjunction with EnergyPlus Generator 2 (EPG2), a UCL in-house Python-based tool for batch producing EnergyPlus v8.0 simulation files (IDF) with variations in built form, building fabric, schedules, environments, and outputs reports. The tool requires building and running Airflow Network-enabled IDFs, and outputting the following values for each timestep:

- Node Temperature (*T*)
- Node Total Pressure (*P*)
- Node Humidity Ratio (kg/kg)
- Linkage Node 1 to Node 2 Mass Flow Rate ($\dot{m}_{1\rightarrow2}$)
- Linkage Node 2 to Node 1 Mass Flow Rate ($\dot{m}_{2\rightarrow1}$)
- Site Outdoor Air Barometric Pressure (*P*)
- Contaminant Emission and Deposition Schedule Value (on/off)
- Zone Air Generic Air Contaminant Concentration (ppm)

PolyPol retrieves the airflow information output from the mass flow rates ($\dot{m}$) between zones, and uses the temperature, pressure, and humidity ratio values to determine the density of air in the zones and contaminant movement through diffusion. Pollution emission and deposition schedules are implemented in the IDF and their values (on/off) are output alongside results. These values are used by PolyPol to inform source and sink schedules, and deposition rate or velocity.

PolyPol then uses an algorithm based on the Generic Contaminant algorithm (page 24, EP Engineering Reference, (DOE, 2013b)) to calculate the indoor concentration of contaminants. Readers are referred to this document for the equation and input parameters. The Generic Air Contaminant Concentration is output as a cross-check to validate the outputs of PolyPol when the indoor environment-dependent decay or emission functionality of PolyPol is not enabled.

### Validation and Influence of Dynamic Internal Temperatures and RH

An initial validation between CONTAM and the EnergyPlus GCM and examination of the influence of dynamic indoor temperatures has been performed by Taylor et al (2013) using the example of $PM_{2.5}$ infiltration into a building. This paper extends that work in order to validate PolyPol and the GCM for internal sources, and examine the vapour-pressure dependent biological decay of influenza.

A single-zoned building (Building 1) was used to validate the PolyPol model against the EnergyPlus GCM and CONTAM. The building (4.0m×5.0m×2.8m) was modelled with infiltration into the building through permeable walls ($3m^3m^{-2}h^{-1}$@50Pa), with the roof and floor considered impermeable. The wall permeability was modelled by applying cracks to the top and the bottom of the walls, modelled with a power law equation using one-way airflow. The flow exponent (n) for both walls was set to 0.66, as per Jones et al (2013). The building envelope was modelled with a U-value of $0.5Wm^{-2}K$.

Influenza was selected as the contaminant for this study, as its survival has been correlated to water vapour concentrations in air (Shaman & Kohn, 2009). The equation (3) describing the relationship between influenza decay and vapour pressure has been used in a previous study examining the impact of humidifiers on virus survival (Myatt et al., 2010):

$$\ln\left(\frac{dN}{dt}\right) = (1.25 \times 10^{-3}) - (1.94 \times 10^{-7}) \times P_v \quad (3)$$

where N is the count of total viable influenza particles and t is time (seconds). This relationship was used to calculate the change in the percent of viable influenza in the air based on the vapour pressure at each timestep predicted by the EnergyPlus model.

Building 1 was simulated with two occupants, one of whom was sick. Influenza has been modelled in previous studies as being both a constant internal source, releasing $1.1x10^{-4}$ infectious influenza viruses per second through breathing, and as a burst source, releasing 0.73 viruses per second when coughing, with 15 one-second coughing episodes per hour (Myatt et al, 2010). Because of the relatively large minimum timestep in EnergyPlus (one minute), the emission of influenza viruses was assumed to have a constant rate over the course of an hour (11.3 influenza viruses an hour), and bursts were not considered. Deposition of influenza viruses was modelled at a rate of $0.0049min^{-1}$ (Nicas & Jones, 2009).

An initial inter-model validation between EnergyPlus GCM, CONTAM, and Polypol outputs was performed. Simulations were run in EnergyPlus, and the dynamic indoor temperature inputs taken from the simulation results model and converted into a continuous value file (.cvf) for CONTAM. Simulations were then run in both CONTAM and EnergyPlus with a reporting time step of 1 minute to minimise the discrepancy between the instantaneous output values of CONTAM and the integrated outputs of EnergyPlus. A Chartered Institution of Building Services (CIBSE) Test Reference Year (TRY) weather file for London Heathrow (CIBSE, 2013) was used for both simulation packages; simulations were run for three weeks in winter (January 1st to January 21st). In addition, PolyPol was run with the influenza decay enabled to demonstrate the influence of vapour pressure on viral persistence. The modelled results of CONTAM, EP GCM, and PolyPol were then compared by fitting a straight line between the results and the r-square for the model agreement calculated.

PolyPol simulations were then run to examine the influence of moisture production, heating, and heat and moisture transport in the building materials on airborne influenza levels. A base case was run without internal sources of heat, moisture, or hygrothermal functionality, while additional models included those with:

1) Heat and Moisture Transport (HAMT) through the building envelope;
2) Moisture production through breathing (40g/hr per person)(BS, 2011);
3) Breathing and HAMT;
4) Breathing and indoor heating to a 20 °C setpoint;
5) Breathing and indoor heating to a 20 °C setpoint, and HAMT;

To model heat and moisture transport, the HAMT heat balance algorithm (Combined Heat and Moisture Finite Element) was enabled. Moisture transport parameters for the different materials was obtained from the WUFI database (Fraunhofer IBP, 2013), with an initial material relative humidity of 60%. Differences in the average maximum airborne influenza count between models were recorded.

**Influence of Retrofits on Influenza levels**

A second building (Building 2) - a 1902-1913 two-storey terrace - was selected from a London building stock model, as the most frequently occurring dwelling (15.4%) and an example of a building which has high retrofit potential (Figure 1). Building 2 was modelled with the same indoor emission rates in the bedroom at night (10pm to 8am), indoor heating schedule, moisture generation, and external weather conditions. Moisture and heat was released into the main bedroom through breathing, while central heating was assumed to operate from 18:00-22:00 and 6:00-8:00. The HAMT algorithm was employed in order to account for the hygrothermal behaviour of the building envelope; material parameters were again taken from the WUFI database.

Building 2 was simulated under both non-retrofit conditions and retrofit conditions, with building fabric U-values taken from earlier work Mavrogianni et al, 2012) for the same building (Mavrogianni, Wilkinson, Davies, Biddulph, & Oikonomou, 2012) (Table 1). Example building permeabilities were selected from CIBSE Guide A (CIBSE, 2006) representing a 'leaky' buildings ($20m^3m^{-2}h^{-1}$) and a 'tight' building ($5m^3m^{-2}h^{-1}$). The differences in influenza concentrations were compared between the models to determine the increase in airborne concentration due to the retrofits.

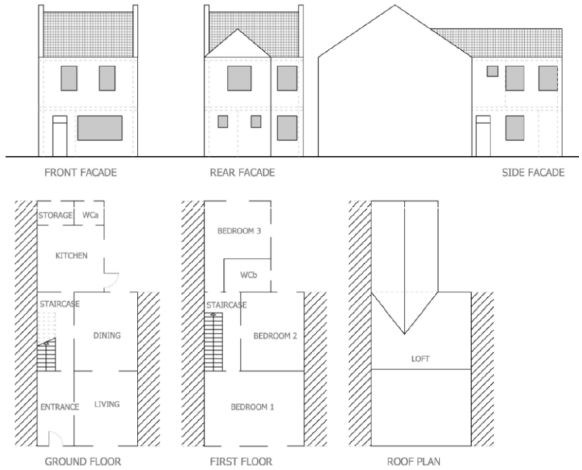


*Figure 1. The terraced house used for the whole-building model (Building 2).*

*Table 1*
*Pre and post-retrofit characteristics of the Building 2 envelope*

| | ELEMENT | PRE-RETROFIT | POST-RETROFIT |
|---|---|---|---|
| U-Values ($Wm^2$)K) | Loft | 0.40 | 0.15 |
| | Floors | 1.20 | 0.51 |
| | Walls | 2.10 | 0.60 |
| | Windows | 4.80 | 2.00 |
| **Permeability ($m^3m^{-2}h^{-1}$@50Pa)** | | 20.0 | 5.0 |

Simulations were run over the same three week period as above, and the differences in viable influenza concentrations during the night periods in the bedroom were compared between models to determine the increase in airborne concentration due to air-tightening.

## RESULTS AND DISCUSSION

### Model Validation

The results of the inter-model comparison in Building 1 show that PolyPol, EnergyPlus GCM, and CONTAM obtain very similar results when the internal temperatures are considered to be dynamic (Figure 2). The coefficient of determination between PolyPol and EnergyPlus GCM was $r^2$=0.999, while between the CONTAM and EnergyPlus models it was $r^2$=0.963. The differences between the CONTAM and EnergyPlus models are attributable to a number of factors. Firstly, CONTAM and EnergyPlus have different methods for calculating wind pressures against the sides of buildings. Secondly, EnergyPlus performs a series of warm-up days, and these can have a slight effect on initial levels during the simulation period. Thirdly, EnergyPlus outputs time-integrated values, while the CONTAM model output instantaneous values. Finally, EnergyPlus requires a volumetric contaminant generation rate, which it converts into a mass generation rate using the zone air density, and then parts per million using a coefficient of $10^6$. Therefore, virus emission must be converted to the volume of air with equivalent mass to the viruses emitted per second. This emission rate is sensitive to the instantaneous air density in the zone, and can lead to differences between the two models particularly when the particle mass is small, as is the case with viruses.

Accounting for the vapour pressure-dependent biological decay of viruses caused a significant decrease in the number of viable viruses in the air in Building 1, reducing the total number by around 50%. Many multi-zonal models and infection risk models assume that contaminants will leave the room or be deposited on surfaces before they become non-viable. These results suggest that the assumption of no biological decay in models may not be entirely accurate. However, models such as the Wells-Riley equation (Riley, 1978) that are based on empirical evidence implicitly account for biological decay.

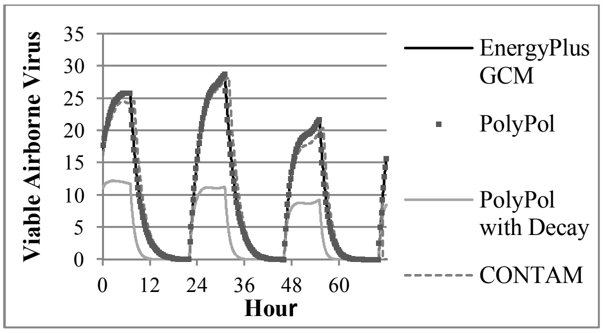


*Figure 2. Indoor numbers of viruses from EnergyPlus, CONTAM, and PolyPol accounting for biological decay for a subset of the simulation period (12am, Jan 19$^{th}$ – 12am, Jan 21$^{st}$).*

The results of simulations with internal heat and moisture sources, and with heat and moisture transport in the fabric of Building 1demonstrate varying levels of influence on the results (Table 2). Alone, HAMT and the addition of moisture through breathing made little difference to the base case, however when indoor heating was included the results reduced by nearly 6% without HAMT and increased 36% with HAMT enabled. This demonstrates the importance of coupled heat and moisture transport on vapour pressure and air density in building simulation models, and consequently airborne influenza levels calculated by PolyPol. Further investigation revealed that the PolyPol-calculated concentration of airborne virus were highly sensitive to the initial moisture content of the walls. These results reflect the high degree of non-linearity in the model.

*Table 2*
*Variations in mean maximum nightime influenza levels between Building 1 model variants.*

| MODEL | VARIATION FROM BASE CASE |
|---|---|
| HAMT | 0.77% |
| Breathing | 0.00% |
| Breathing + HAMT | 0.77% |
| Breathing + Heat | -5.96% |
| Breathing + Heat + HAMT | 35.5% |

### Influence of Retrofits on Influenza Levels

Influenza levels were elevated in Building 2 following retrofit, due to the reduced ventilation. There was little difference in the indoor vapour pressure observed between the models during the simulation period, meaning ventilation rate is likely the main driver of the differences between the pre- and post-retrofit terraces. The average bedroom infiltration air change rate (ach) during the simulation period for the non-retrofit Building 2 was 0.22ach, while the retrofit Building 2 had an infiltration air change rate of 0.05ach.

The number of viable viruses in the air can be seen in Figure 3. The results indicate that air-tightening of dwellings may increase the risk of disease transmission during periods of particularly low outdoor wind speed. In comparison to the results for Building 1 (Figure 2), the count of viable airborne influenza is quite low. This is due to the higher permeability of Building 2 ($5m^3m^{-2}h^{-1}$ and $20m^3m^{-2}h^{-1}$) versus Building 1 ($3m^3m^{-2}h^{-1}$) and the modelling of airflow out of the bedroom and through the rest of the building. The results suggest that the risk of airborne transmission of influenza is relatively low in typical dwellings, and that transmission may occur largely through large droplets and direct contact.

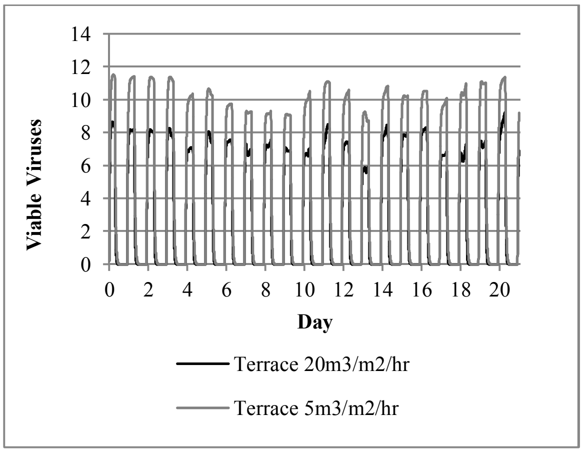


*Figure 3. The differences in viable flu counts following air tightening of the terrace.*

The results suggest that retrofitting existing properties in order to meet energy saving goals may increase the risk of airborne disease transmission in the future by reducing the passive exchange of air, particularly if appropriate alternative means of controllable ventilation are not provided. However, retrofits may also result in buildings becoming warmer, with potentially more water vapour inside due to a reduced ability to remove moisture generated through indoor activities and breathing; this would act to accelerate biological decay of influenza. The complex relationship between the survival of airborne biological contaminants and indoor temperature and humidity levels may mean that building retrofits may alter the profile of contaminants that pose the largest risk to building occupants.

It is important to note that, while indoor air quality and risk of airborne disease transmission may increase when buildings have been retrofitted, other causes of morbidity and mortality such as those caused by exposure to cold, may decrease.

The models employed represent a simplification of the true nature of airborne influenza release. The sizes of aerosols and droplets were not considered, and all aerosols were considered to have the same deposition rate. In reality, large droplets will fall to the ground quickly, while smaller droplets and aerosols will remain suspended for longer. Furthermore, multi-zonal models assume that a zone is well-mixed and are not able to account for proximity between infected individuals in a room. The low levels of virus counts, and the relatively rapid decay in the indoor air predicted by this model suggests that airborne transmission is unlikely to be a significant contributor to the infection transmission pathway, however further research is required to better understand the dynamics of influenza transmission.

EnergyPlus offers an advantage over CONTAM in that it is able to take into account the dynamic thermal behaviour and moisture buffering performance of the building envelope, which influences the indoor temperature and RH, and therefore the density of air. Under certain scenarios, as demonstrated above, this can impact on indoor concentrations of pollutants. PolyPol offers a further advantage over the EnergyPlus GCM, in that it can model multiple pollutants, and can account for the conditions of the indoor air on the deposition rate or biological decay of a contaminant.

PolyPol is intended as a tool to expand the capabilities of the EnergyPlus GCM, and there are a number of limitations to PolyPol when compared to CONTAM. These include:

- A small minimum timestep of 1 minute cannot account for short contaminant emission bursts (e.g. coughing).
- The program reads output files from EnergyPlus, which detail temperatures, pressures, and vapour pressures and airflow between the nodes for each timestep; for more complex buildings, or for long simulation periods, this can create large and unwieldy files.
- PolyPol and EnergyPlus GCM output contaminant concentrations in parts per million (PPM), which needs conversion to units more commonly associated with particulates (e.g. mass per unit volume, # per unit volume).
- EnergyPlus models require the implementation of the Airflow Network, which is complex and time-consuming if an IDF generator is not used.
- The EnergyPlus GCM uses a predictor-corrector algorithm, which allows building operation to be influenced by contaminant levels. PolyPol is implemented in post-processing, and so is not able to feedback to building operation. Consequently, PolyPol is unable to be used to model Indoor Air Quality (IAQ)-controlled operation of ventilation systems.

While this paper has focused on the ability of PolyPol to model biological decay, the tool may also be used to estimate changes to contaminant concentrations due to temperature or humidity-dependent chemical reactions and deposition and building penetration factor. In addition, PolyPol has the ability to predict the concentrations of multiple contaminants simultaneously, with the benefit of reducing the number of required simulations in multi-pollutant studies.

## CONCLUSIONS

PolyPol is, to our knowledge, the first tool, which combines whole-building airflow modelling, dynamic thermal simulations, hygrothermal models, and biological models to estimate the pathogen concentration in indoor air. Further work can investigate the increase in the risk of disease transmission due to the air-tightening and retrofitting of the UK housing stock.

## NOMENCLATURE

| | |
|---|---|
| $\Delta P$, | pressure difference across airflow path (Pa); |
| $P_1, P_2$, | absolute pressures on either side of the airflow path (Pa); |
| $\rho$, | density of air (kg/m$^3$); |
| $v_1, v_2$, | entry and exit velocities of the air (m/s); |
| $g$, | acceleration due to gravity (9.8m/s$^2$); |
| $z$, | airflow path elevation (m); |
| $P_d$ | pressure of the dry air component (Pa); |
| $P_v$ | water vapour pressure (Pa); |
| $R_d$ | specific gas constant for dry air (J/kg/K); |
| $R_v$ | specific gas constant for water vapour (J/kg/K); |
| $T$ | temperature (K); |
| $t$ | time (seconds). |

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