A PARTIAL REVIEW OF MASS BALANCE MODELS

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Mass balance models are deterministic models, derived from understanding of the underlying physical processes that govern transfers and transformations of pollutants in the environment. They are the main method used in indoor air modelling to provide a relatively simple means of predicting indoor pollutant concentrations both spatially (e.g. in different buildings or rooms) and over time. Often they are applied on the assumption that the rooms or buildings under study represent well-mixed air volumes, in which steady state conditions prevail. As such, they are especially useful tools for estimating changes in average pollution levels as a result of variations in indoor emission sources or ambient concentrations.

The simplest approach to mass balance modelling is provided by the single-zone technique, which takes into account airflow between only one or two compartments. The models have generally been based on the assumption of well-mixed air existing in each zone, microenvironment, group of microenvironments, or the whole building, and under these conditions they appear to perform well, giving results consistent with those from experiments or field measurements. Because the processes they represent are to some degree time-dependent, however, most single-zone mass balance models are at least partially dynamic in form - or can be applied to simulate time-varying conditions over time-scales longer than those required to ensure complete mixing.

A more complex approach is provided by multi-zone models. These consider a building to comprise several well-mixed zones, connected by airflow between them. Amongst others, examples include COMIS (Feustel 1999) and CONTAM (Walton 1997, Dols et al. 2000). A further, complex multi-zone model, COwZ (Stewart & Ren 2006), was developed to predict
mass transfer and pollutant dispersion with regard to spatial and temporal variations in an individual room. It is, in practice, a hybrid between multi-zone and computerised-fluid dynamic (CFD) techniques. The CowZ model is based on the COMIS model while dividing individual rooms into separate microenvironments, using a Cartesian grid.

Mass balance models are based on the law of conservation of mass/matter (the Lomonosov-Lavoisier law), which states that “mass of a closed system of substances will remain constant over time, regardless of the processes acting inside the system”. In other words, it can be said that “mass can neither be created nor destroyed, although it may be rearranged in space, and changed in form”. This basic form of mass-balance model can be expressed as an ordinary differential equation:

$$\frac{dC}{dt} = C_{\text{Sources}} - C_{\text{Sinks}}$$


Equation 1

where $C$ is concentration at time $t$,

- $C_{\text{Sources}}$ is sum of concentration gain from all sources, and
- $C_{\text{Sinks}}$ is sum of concentration loss from all sinks.

Equation 1 can be used in indoor air pollution studies to predict indoor concentrations under specified emission or removal processes. It can, for example, be adapted and expanded to represent the range of different factors that affect indoor particulate concentrations. With an assumption of a well-mixed condition in a naturally-ventilated room with similarity of temperatures between indoors and outdoors, the mass balance model can thus be written as (Nazaroff, 2004, Thatcher et al., 2003):

$$\frac{dC_i}{dt} = (\lambda + \lambda_L)PC_o + (\lambda_a + \lambda_{La})P_aC_{ia} - (\lambda + \lambda_L + \lambda_a + \lambda_{La} + \beta)C_i + R + F + K + X$$


Equation 2

Where $t$ is time (h),

- $C_i$ is indoor concentration at time $t$ (mass/volume),
- $C_o$ is outdoor concentration at time $t$ (mass/volume),
Due to differences in the properties of different pollutants, and the varying importance of the processes operating in different indoor environments, there is no individual mass-balance model that can cover all circumstances (Nazaroff, 2004). A number of studies have tried to represent the processes involved in rather different formulations of the mass balance model (Hussein & Kulmala, 2008, Nazaroff, 2004, Wallace, 1996): for example, for particulates (PM) (e.g. Dimitroulopoulou et al., 2006, Kulmala et al., 1999, Riley et al., 2002, Schneider et al., 2004, Thornburg et al. 2001), elemental PM (e.g. Alzona et al., 1979, Lunden et al., 2003, Raunemaa et al., 1989) and other pollutants such as CO, NO₂, Rn, VOCs, and O₃ (e.g. Li & Niu, 2007, Nazaroff & Cass, 1986).

Raunemaa et al. (1989) developed an indoor concentration model:

$$\frac{dC_i}{dt} = \lambda PC_i - (\lambda + \beta)C_i + f(\beta, C_i, t_a) + I$$  \text{Equation 3}

where $f(\beta, C_i, t_a)$ is the so-called functional re-emission rate (mass/volume/time), and $t_a$ is accumulation time. The model considered outdoor PM (monitored at air intake) and simulated...
its transportation indoors through mechanical ventilation, where deposition and re-suspension occur. Cooking activity was not included in the model due to its infrequent occurrence. Model simulations were done under steady-state conditions for fine-mode sulphate particles, based on deposition experiments of different element particles and particle mass carried out at an office and an apartment in Helsinki. In the validation of the office data, air exchange rates were calculated from tracer-gas measurements, while the penetration factor, deposition rate and resuspension rate were obtained from the experiments. Good agreement was found between the predicted and monitored I/O ratios (though $R^2$ was not supplied).

Kulmala et al. (1999) applied an indoor time-varying model (with 10-min time step) to predict indoor surface accumulation and indoor air concentration of chemically inert particles with relatively constant size distribution:

$$\frac{dC_i}{dt} = \lambda PC_i - (\lambda + \beta)C_i + \Delta C_i + I_i$$  \hspace{1cm} Equation 4

where $I_i$ is generation or loss from indoor sources/sinks (mass/volume/time). The model was run for radioactive aerosols, traffic-derived PM, and constant emission from an indoor source, but no validation carried out. Model performance was, however, compared with that of the Raunemaa et al. (1989) model, by using the same data set of indoor fine-mode sulphate particles, with a slightly different penetration factor and resuspension rate, and results were claimed to be consistent, though neither derivations of these adjusted variables nor $R^2$ were reported.

Schneider et al. (2004) developed and applied a model to predict concentrations of PM in the size range 0.5-4µm inside an unoccupied mechanically-ventilated apartment in Copenhagen. The model was:
\[
\frac{dC_t}{dt} = (\lambda_t - \lambda_{M,t})P + \lambda_{M,t}C_o - (\lambda_t + \beta)C_t
\]

Equation 5

where \( \lambda_t \) is air exchange rate at time \( t \) (/time), \( \lambda_{M,t} \) is air exchange rate through mechanical ventilation at time \( t \) (/time), and \( \lambda_t - \lambda_{M,t} \) is air infiltration rate through leakages at time \( t \) (/time).

The model was run using a 30 minute time-step, and with monitoring data collected over autumn, winter, and spring for a month period each. The outdoor concentrations were monitored at the building façade. The penetration factor was obtained from experiments, whereas, deposition rate was adapted from the literature. Air exchange rates were estimated from tracer-gas experiments, while mechanical ventilation rates were estimated from monitored air pressure differences.

The model was considered to perform reasonably well, predicted values tracking the peaks and troughs relatively closely in autumn, and the scattergrams suggested agreement between the predicted and observed values in both autumn and spring. Performance was less good in winter, when the air exchange rates were low. Neither \( R^2 \) nor SEE was reported, but instead the model was evaluated on the basis of the ratios of median values between the predicted and observed concentrations. Attempts were also made to enhance the model using stepwise regression analysis to incorporate relevant measured variables (routine wind speeds, air exchange rates, and outdoor relative humidity). The adjusted model thus obtained was considered to improve model performance, though again no independent validation was done. The adjusted model also involves some degree of ‘double-counting’ because the variables such as outdoor wind speed and air exchange rates were already embedded in the initial mass-balance model.

Thornburg et al. (2001) presented models predicting indoor PM concentrations for buildings which either had HVAC systems or were naturally ventilated, in the US. The model for buildings with HVAC was:
where $Q_L$ is volumetric airflow rate from infiltration through leakages (length/time), $Q_M$ is volumetric airflow rate from the HVAC (heating, ventilation, and air-conditioning) system (length/time), $C_M$ is concentration from the HVAC system (mass/volume), $Q_{Lx}$ is volumetric airflow rate from exfiltration through leakages (length/time), $Q_{Mr}$ is volumetric air-return flow rate from the room to the HVAC system (length/time), $Q_{Ms}$ is volumetric airflow rate to the outdoors through exhaust (length/time), and $i$ is indoor generation/emission rate (mass/time).

This HVAC model was also expanded into two versions, one for commercial buildings and the other for residential buildings. For naturally-ventilated dwellings, their final model was:

$$C_i = (C_{i,t=0} - C_{i,t=n}) \exp[-(\lambda + \beta)t] + C_{i,t=n}$$  \hspace{1cm} \text{Equation 7}$$

and

$$C_{i,t=n} = \frac{\lambda PC_o + i}{\lambda + \beta}$$  \hspace{1cm} \text{Equation 8}$$

where $C_{i,t=0}$ is initial concentration (mass/volume) and $C_{i,t=n}$ is final or steady-state indoor concentration (mass/volume). If the integration time is large enough to make the exponential term substantially less than 1, steady-state conditions, where $C_i = C_{i,t=n}$ can be assumed (Thornburg et al., 2001).

Parameterisation was done by imputing values for each parameter from the literature and professional judgments. Monte Carlo simulation - a probabilistic method - was used to randomly generate the model variables with user-defined probability distribution functions. Sensitivity analyses were also undertaken to compare I/O ratios for different types of building and ventilation, as well as estimate penetration factors for particles in different size ranges. Independent validation was not undertaken but the findings were compared with those in the literature.
A probabilistic approach was also used by Dimitroulopoulou et al. (2006) to simulate variables in the INDIAR model:

\[
\frac{dC_i}{dt} = \lambda PC_o + \lambda_a C_{ia} + \lambda_b C_{ib} - (\lambda_a + \lambda_b + V_a \left( \frac{S}{V} \right)) C_i + \frac{i}{V}
\]

Equation 9

where \( C_{ib} \) is indoor concentration in adjacent room \( b \) at time \( t \) (mass/volume) and \( \lambda_b \) is air exchange rate room \( b \) (/time). The model predicts the indoor concentration in a room, on the basis of outdoor concentration, indoor generated concentration and indoor concentrations from the two adjacent rooms. Outdoor concentrations of NO\(_2\), CO, PM\(_{2.5}\) and PM\(_{10}\) were obtained by taking the geometric means from five routine monitoring stations in the UK (Harwell, Birmingham East, Bradford, Bloomsbury and Marylebone Road), whilst air exchange rates were assumed from air infiltration rates. All other variables were obtained from the literature with user-justified distribution functions. Sensitivity analysis was undertaken to identify the effects of the variables on indoor concentrations and predicted concentrations were compared both between the pollutants and with the monitored outdoor concentrations. I/O ratios and 24-hour average concentrations from the modelling were also compared with results in the literature, though no validation was carried out.

As these studies indicate, previous attempts at developing mass balance models have largely been small in scale, and applied for only short periods of time and a small numbers of locations. Models that have been developed for larger scale studies have tended to use parameter estimates derived from literature or national statistics. In neither case, has independent validation usually been carried out, and few (if any) of the models have been used for practical studies.
References


