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COMPARISON OF DIFFERENT METHODS OF INCORPORATION OF STOCHASTIC FACTORS INTO DETERMINISTIC MODELS OF INDOOR AIR QUALITY

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SYNOPSIS

The paper will discuss problems connected with incorporation of stochastic factors into deterministic models of indoor air quality. Three different methods:

- quasi dynamic multi-zone modelling with generating of input data time series,
- multi-zone modelling based on the theory of stochastic differential equations,
- Monte-Carlo simulation with independent random generating of stochastic parameters,

will be shortly presented. Described methods are compared on the base of computer simulation of CO_2 concentration in simple two compartment office. The comparison of simulation outcomes shows that the way of stochastic disturbances incorporation into indoor air quality models does not have an important influence on mean value of predicted concentration. At the same time the analysis of standard deviations indicates that the method of disturbances generation and its later incorporation have a great influence on probability distribution of estimated concentrations. The author would like to highlight that differences. The conclusions include also subjective opinion of the author on main advantages and disadvantages of each of proposed methods.

LIST OF SYMBOLS

C - contaminant concentration matrix,
C_i - concentration of contaminant in zone i,
F - the drift matrix; the terms of the matrix are the constant part of coefficients K_i.
G - the diffusion matrix,
K_i - coefficient characterising transport of contaminants between zones or mixing factors, last coefficient in each row represents such mechanisms as production or removal of the pollutant in a zone.
n - number of equations that have to be solved to achieve solution of SDE,
N - number of zones in the building,
t - time,
ξ - the Gaussian white noise variables matrix.

1. INTRODUCTION

The experiences from many measurement programmes indicate that proper explanation of Indoor Air Quality level and dynamics of its variability should include also a description of many disturbances of stochastic nature. There are number of such disturbances but the interactions between weather fluctuations and/or occupants activities and building characteristics (including ventilation and air conditioning systems) may be regarded as the most important examples of these random factors.

As neglecting of these phenomenon may lead to a great inaccuracy there is a need to develop new reliable indoor air quality prediction tools and calculation methods that allow to take randomness of pollutant migration process into account. In last few years several new methods have been proposed by different research centres all over the world. Although, all these methods are based on conventional deterministic multi-zone models of pollutant migration in buildings, they differ in methods of random factors incorporation into the model. The paper will concentrate on the following methods:

- generating of disturbances' time series and than multiple multi-zone simulation,
- description of disturbances as Gaussian distributions and application of SDE theory,
- multiple generation of set of input data and than application of Monte-Carlo simulation.

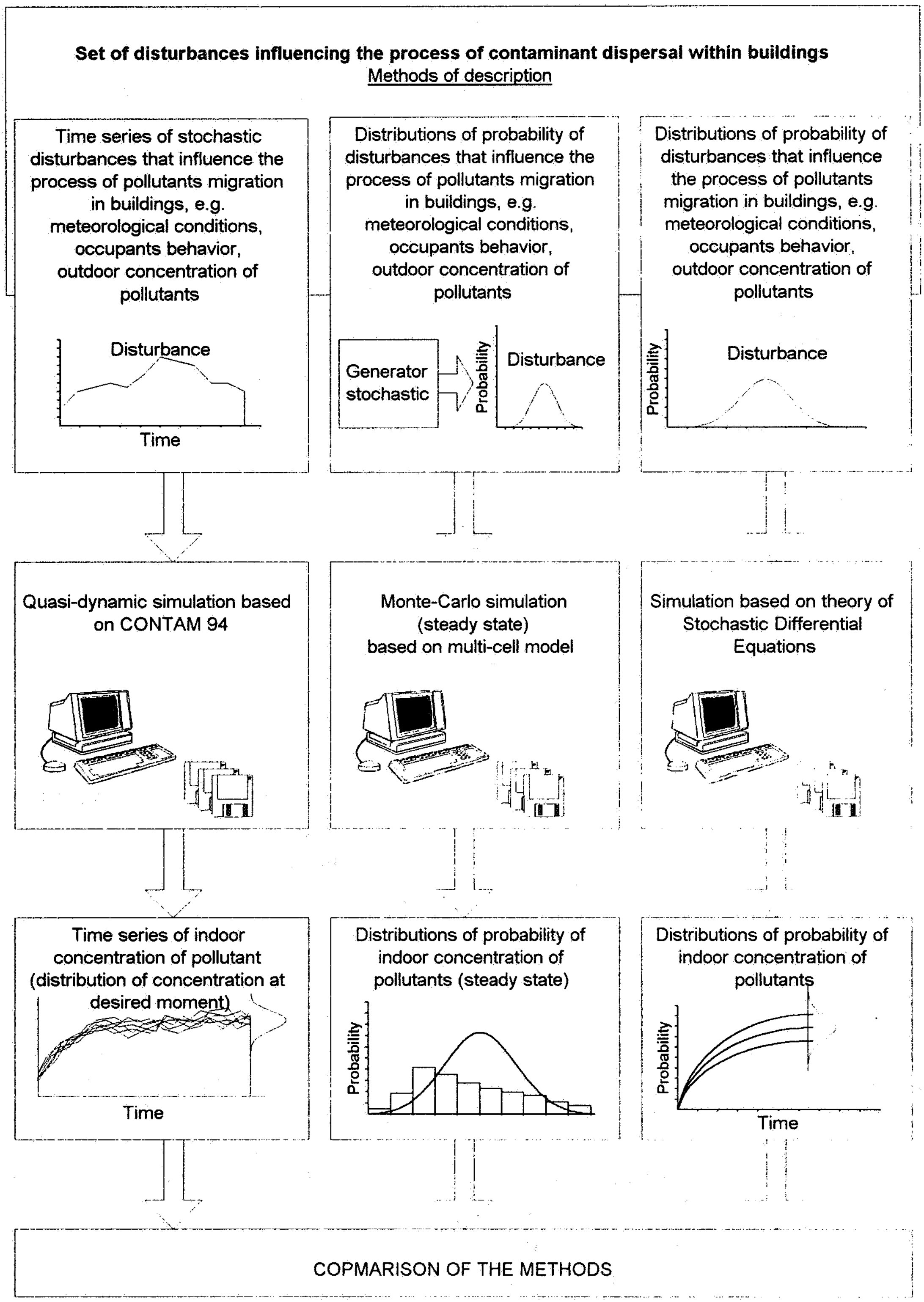


Figure 1. Comparison of different methods of incorporation of stochastic factors into deterministic models of indoor air quality. The scheme of applied methodology.

2. MULTI-ZONE DETERMINISTIC CONTAMINANT DISPERSAL MODELS

The most popular tool for contaminants' dispersal modelling in buildings are models based on deterministic approach. That type of models assumes perfect understanding of cause-to-effect chains in physical processes (different forms of energy and mass transport in buildings). Generally, the process of contamination dispersal is inseparably connected with two other main tasks: thermal analysis and air flow analysis. Often in practical applications thermal and air flow analysis are substituted by simple steady state models or specified fields of temperature and air flows [1]. Usually, for the purpose of modelling, selected building is described as a network, where nodes (called also zones) represent the volumes to which assumption on uniformity of parameters can be made (zones may represent groups of rooms, rooms, portions of rooms, shafts or portions of air handling systems) [7]. That simplification allows to write a set of ordinary differential equations based on contaminant mass balance,

$$\begin{bmatrix} \frac{dC_1}{dt} & = & K_1C_1 & + & K_2C_2 & + \cdots + & K_NC_N & + & K_{N+1} \\ \frac{dC_2}{dt} & = & K_{N+2}C_1 & + & K_{N+3}C_2 & + \cdots + & K_{2N+1}C_N & + & K_{2N+2} \\ \cdot & = & \cdot & \cdot & \cdot & \cdot\ \cdot\ \cdot & \cdot & \cdot & \cdot \\ \cdot & = & \cdot & \cdot & \cdot & \cdot\ \cdot\ \cdot & \cdot & \cdot & \cdot \\ \cdot & = & \cdot & \cdot & \cdot & \cdot\ \cdot\ \cdot & \cdot & \cdot & \cdot \\ \frac{dC_N}{dt} & = & K_{N^2}C_1 & + & K_{N^2+1}C_2 & + \cdots + & K_{N^2+N-1}C_N & + & K_{N^2+N} \end{bmatrix} \quad (1)$$

Investigator is usually looking for discrete solution of formulated set of equations. Number of equations is equal to number of selected zones. Of course if simultaneous air flow or/and thermal analysis is performed number of equations will increase. A lot of computer programmes built on that type of models have been developed.

3. INCORPORATION OF STOCHASTIC FACTORS INTO POLLUTANTS MIGRATION MODELS

3.1. Generating of input data time series for quasi dynamic multi-zone models

The simplest way of incorporation stochastic factors into deterministic models is to substitute constant values of input data by real or simulated time series of the possible states of modelled parameter. The option that allow to prepare some input data as time series became a standard in new generation of contaminant dispersal software. That improvement refers not only to data directly connected with contaminants as:

- emissions and sinks of contaminants,
- concentrations of contaminants in surroundings,

but also to data influencing the process of air flows like:

- meteorological factors (atmospheric pressure, temperature, humidity, velocity and direction of wind),
- occupants behaviour (door and windows opening, switching ventilation systems).

Decreasing of time step brings performed simulation nearer to reality. From the other hand, very small time steps cause considerable increase of computing time.

3.2. Description of stochastic factors as Gaussian white noise for SDE technique

In the late eighties and early nineties scientists from Canada published several papers ([2], [3], [4], [5]) on application of Stochastic Differential Equations (SDE) to the modelling of contaminant dispersal in buildings. Assumption that the K_i factors (in equation 1) may have random nature as well as application of SDE technique cause that equation 1 may be rewritten as

$$\frac{d\mathbf{C}}{dt} = \mathbf{F}(\mathbf{C}) + \mathbf{G}(\mathbf{C})\xi \qquad (2)$$

Now, solution of set of equations is more complex. Solving the SDE using either *Itô* or *Stratanovich* interpretation will result in a set of possible results. The specific solution $C_i(t)$ depends on assumed probability. Moreover, the number of equations to solve depends on second power of zones number

$$n = \frac{N(N+1)}{2} + N \qquad (3)$$

3.3. Generating set of random factors for Monte-Carlo simulation

Another way to incorporate randomness of some processes into deterministic models is multiple generation of set of possible input data from a data space (known parameters of standardised distributions; M-C or known empirical distributions; M-C(de)) and than application of Monte-Carlo simulation. Of course Monte-Carlo simulation is performed on a base of deterministic multi-zone models (steady state or dynamic). One should note that the accuracy of Monte-Carlo method is dependent only on number of runs (after 60-80 improvement of the accuracy is very small) and does not depend on number of input parameters.

4. COMPARISON OF THE METHODS

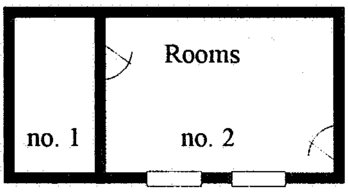
To present, how the selection of method results in differences in simulation outcomes, special computer test of CO_2 concentration in simple two compartment office was performed. The comparison was carried out assuming that the office (characteristics briefly presented in table 1) is ventilated in either natural or mechanical way. Simulation included the randomness of:

- weather fluctuations(conditions of Polish climate in winter),
- concentration of CO_2 in surroundings and
- occupants activities (entering and leaving the office, opening of door and windows, switching ventilation systems on and off).

Of course the set of disturbances influencing the indoor air quality in office was the same for all cases. Differences refers to method of its description and further incorporation into simulation model.

Results achieved by the quasi dynamic multi-zone modelling with generating of input data time series (10 simulations for different set of time series) using CONTAM94 [7] is presented at figure 2. Outcomes from simulation based on SDE is presented at figure 3. Figure 4 presents the example of steady state Monte-Carlo simulation. Figures 2,3,4 present the results from wider analysis of influence of stochastic disturbances on process of pollutant migration inside buildings carried out by *Sowa* [6].

Table 1. Characteristics of simple two compartment office.

	**Room 1** additional room	**Room 2** main office
Floor area	15 m^2	50 m^2
Volume	45 m^3	150 m^3
Number of occupants	variable from 0 to no. of occupants present in office	variable from 0 to 10
Openings	door to room 2 (+comp. grill)	entrance door, 2 windows, door to room 1 (+comp. grill)
Ventilation systems (options)		**Pollutants**
<u>mechanical ventilation</u> supply: r. 1, 450 m^3/h (3 h^{-1}) r. 2, 0 m^3/h exhaust: r. 1, 315 m^3/h r. 2, 135 m^3/h recirculation: outdoor air 300 m^3/h return air 150 m^3/h windows closed	<u>natural ventilation</u> in each room 1 shaft 0.14 x 0.14 m height 1 m estimated characteristics $\Delta P = 1$ Pa W = 50 m^3/h $\Delta P = 4$ Pa W = 100 m^3/h windows open randomly	<u>pollutant: CO_2</u> source: occupants intensity of emission: 20 l/h per person, initial concentration: 780 mg/m^3 (~340 ppm) CO_2 outdoor concentration mean 780 mg/m^3 SD 20 mg/m^3

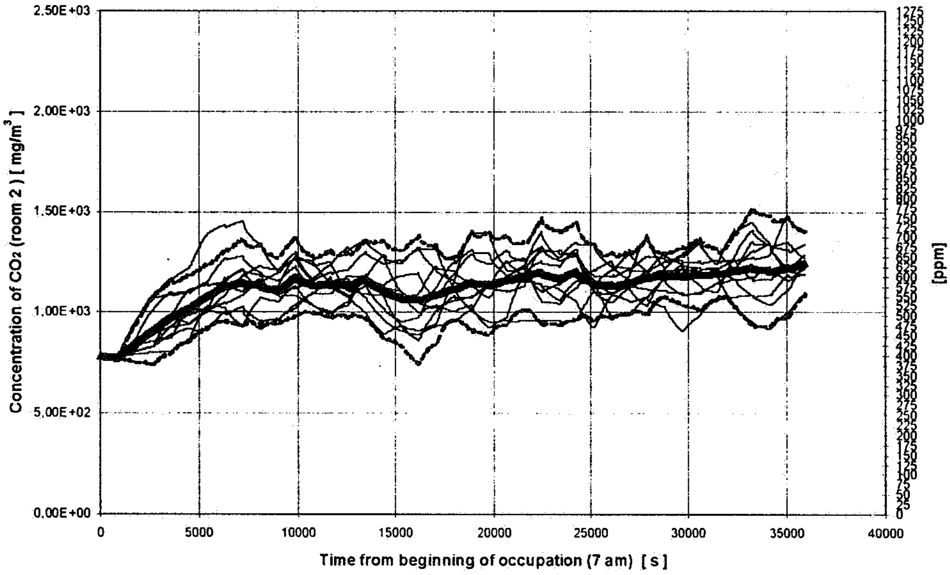


Figure 2. Concentrations of CO_2 in room 2 ventilated mechanically (thin lines - 10 independent runs, thick line - mean value, thick dashed lines - mean value with two standard deviation margin), [6]. Simulation based on generating of disturbances' time series and than multiple simulation using quasi dynamic multi-zone model of air pollution migration in buildings CONTAM94, [7].

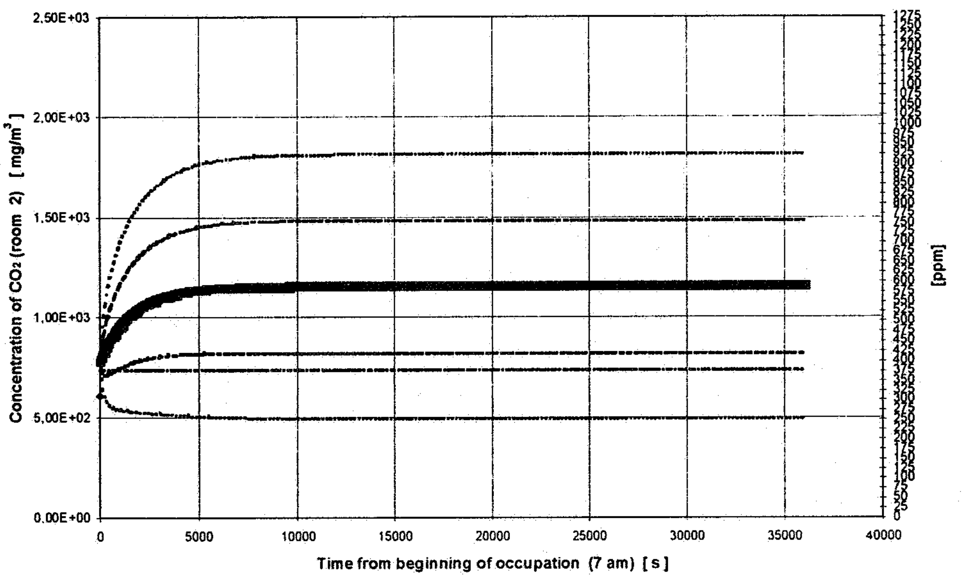


Figure 3. Concentrations of CO_2 in room 2 ventilated mechanically (thick line - expected value, thick dashed lines - expected value with one and two standard deviation margin), [6]. Simulation based on description of stochastic disturbances as Gaussian distributions and than application of stochastic differential equations (SDE) technique.

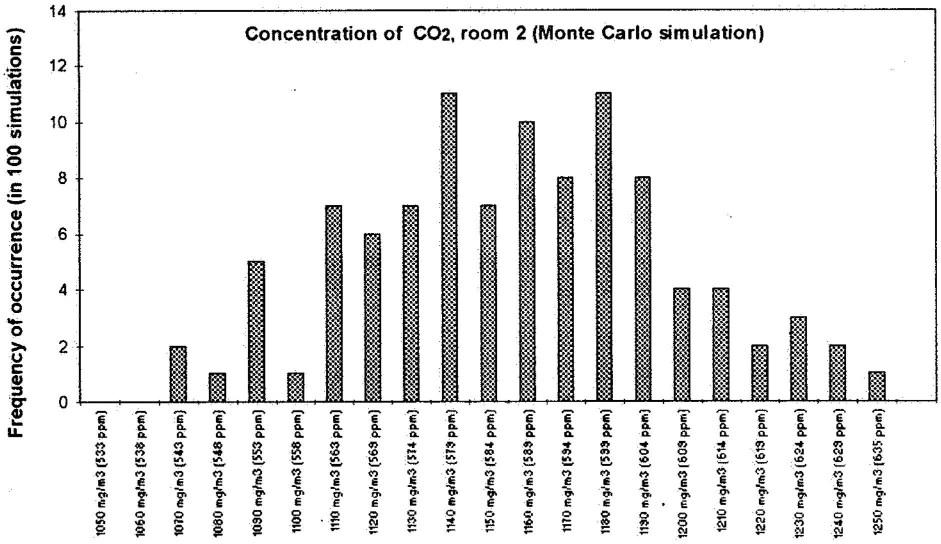


Figure 4. Frequency of CO_2 concentrations in room 2 (mechanical ventilation). Monte-Carlo simulation based on 100 independent generations, [6].

The mean values and standard deviations of simulated concentrations for described simple test office are presented at table 2. CONTAM denotes simulation based on generating of disturbances' time series and than multiple simulation using quasi dynamic multi-zone model of air pollution migration in buildings CONTAM94. Simulation based on description of stochastic disturbances as Gaussian distributions and than application of stochastic differential equations technique was signed as SDE. Monte-Carlo analysis was performed for generation of set of possible input data based on both known parameters of standardised distributions; M-

C, and known empirical distributions; M-C(de). Monte-Carlo simulations were based on 100 independent generations.

Table 2. The comparison of simulation results for proposed methods.

The method	CO_2 concentration [mg/m^3]							
	Mechanical ventilation				Natural ventilation			
	Room 1		Room 2		Room 1		Room 2	
	Mean	SD	Mean	SD	Mean	SD	Mean	SD
CONTAM	1290.58	181.56	1146.37	95.65	1319.06	228.83	1156.07	147.73
SDE	1306.45	429.07	1154.97	329.70	1290.47	539.20	1133.04	573.00
M-C	1235.99	512.64	1077.28	432.24	1339.95	1257.51	1171.14	1180.49
M-C (de)	1296.03	64.46	1152.20	40.36	1302.60	114.98	1146.24	94.87

4. CONCLUSIONS

The comparison of simulation outcomes shows that the way of stochastic disturbances incorporation into contaminant migration deterministic models does not have an important influence on mean value of predicted concentration (table 2). At the same time the analysis of standard deviations, presented in table 2, indicates that the method of disturbances generation and its later incorporation into contaminant dispersal model results in great differences in distribution of estimated concentrations.

The highest values of standard deviation of concentration occurred in cases when generation of random input data is performed on a base of known parameters of standardised distributions (especially when disturbances are treated as independent factors). This methods seem to overestimate variability of contaminant concentrations. One should notice that using that methods, it is possible to reach unrealistic values of concentrations (e.g. negative concentrations) with quite high probabilities. Monte-Carlo method based on empirical distributions and quasi dynamic modelling based on description of disturbances as interrelated time series provide lower values of standard deviation.

All these differences are much higher for cases when natural ventilation is considered. It is the result of option that allow to open the windows. Windows opening very strongly and very rapidly influence the concentration of pollutants. Moreover in that case description of air volume as one of well known distributions is difficult and questionable.

Mean and SD of CO_2 in Room 1 which is ventilated indirectly, by air from room 2, are higher.

That simple test indicates that outcomes of the multi-zone simulations are very sensitive to method of stochastic disturbances description. At the moment, it is quite difficult to definitely say that one of proposed method is simply the best (however is seems to be more safe to recommend Monte-Carlo method based on empirical distributions and quasi dynamic modelling based on description of disturbances as interrelated time series). All methods have their advantages and disadvantages (table 3).

One may expect that in near future that type of modelling will be more popular. Risk analysis calls for probability distributions of concentrations. Incredibly fast development of computer science and technology will probably overcome some of these disadvantages. So, it seem to be quite good time for discussion on the best methods to incorporate randomness of several processes into indoor air modelling.

Table 3. Main advantages and disadvantages of presented methods.

Method	Main advantages	Main disadvantages
Time series and quasi dynamic simulation	• correlation between different parameters may be taken into account, • existing software may be applied (contaminant migration simulators, weather generators, etc.)	• time consuming description of building, • high hardware requirements (simulation of real building with small time step), • demands for huge computer memory to store simulation results,
modelling based on SDE technique,	• modern approach, • results of analysis presented as probability distributions,	• lack of user friendly software, • time consuming calculations, • high hardware requirements, • unrealistic values of concentrations may be reached (e.g. negative concentrations) with quite high probabilities,
random data generating for M-C simulation.	• simplicity of the method, • existing software may be applied (contaminant migration simulators, etc.), • relatively short time of computing,	• treating input data as independent parameters, • unrealistic values of concentrations may be reached (e.g. negative concentrations) with quite high probabilities,

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