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...door Air Quality Modeling Workshop Report

Preston E. McNall

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
National Engineering Laboratory
Center for Building Technology
Building Physics Division
Gaithersburg, MD 20899

April 1985

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Prepared for
Environmental Protection Agency (MD-75)
...onmental Monitoring Systems Laboratory
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U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

INDOOR AIR QUALITY MODELING WORKSHOP REPORT

Preston E. McNall

ABSTRACT

Comprehensive modeling of emission, absorption, movement and controls of indoor air contaminants is essential for developing national policy for IAQ assessment and controls. This report describes several topics discussed in the workshop on indoor air quality, which was held on February 11, 1985 at the National Bureau of Standards. Researchers on IAQ modeling were invited to state their current activities, identify research needs and recommend specific parameters and contaminants to be included in the models. The input thus obtained in this workshop will be incorporated into an advanced simulation model for IAQ, to be developed by NBS under a contract with EPA.

KEY WORDS:

absorption; air circulation; contaminants; emission; indoor air quality; simulation models

IAQ Modelling Workshop Report

February 11, 1985

at the National Bureau of Standards

The National Bureau of Standards, Center for Building Technology has a project funded by the Environmental Protection Agency IAG DW13931103-01-0, for the purpose of establishing a framework for an extensive IAQ model to predict the levels of indoor pollutants under various conditions. In order to receive the available technical inputs, an invited workshop was held. Each of the participants was asked to state briefly what he is currently doing in the modeling area, and to contribute one or more recent publications.

While all of the experts involved in indoor air quality modelling research could not attend, those who did were familiar enough with prior work so that all important facets of the problem were covered. Other modellers who may have specific inputs were identified, and other information will be obtained by literature search or personal contact.

The meeting attendance and a list of the recent publications are appended to this report.

The meeting began with a welcome by Dr. Preston McNall and introduction of the attendees. Also attached is a list of handouts brought by the participants.

Dr. Mage of EPA stated that a good comprehensive model is needed to:

1. Evaluate the effectiveness of various IAQ control options, such as ventilation, purification and the use of heat exchangers in terms of energy conservation, indoor thermal comfort, material degradation and cost/benefit analysis.

2. Evaluate the value of various test data collected for emission rate, sink strength and diffusion rate.

3. Coordinate research programs by identifying key parameters to be studied.

4. Evaluate the requirements for testing instruments, e.g., the right instrument time constant to measure a given parameter, when to measure, how often, etc.

5. Check the measured contaminant concentration data with respect to air flow patterns and the temperature stratification around the instruments.

6. Be able to create a scenario whereby different people using different models can yield consistent answers.

7. Predict microenvironmental distribution of pollutant concentration, which will dictate the sizes of space and time increments for experimental measurements.

8. Determine the value of data collected for other purposes for model validation.

9. Be able to evaluate unpublished and/or obscure data sets.

10. Be able to lead to the establishment of standards.

11. Be used for the risk assessment for various pollutants by being able to predict their peak exposures which may occur in a short time period in a microenvironment. (The model must be able to predict microenvironmental pollutant concentration distribution.)

Dr. Moshandreas of IITRI recently completed a study on source/sink strengths of the combustion products of furnaces, ranges, stoves, gas heaters, kerosene heaters, gas dryers, and cigarettes. His laboratory is engaged in testing proprietary pollutant control methods. He also studied "sick building" problems and is developing an expert system to assist local authorities for developing counter measures.

His model is based upon a mass balance method and incorporates a Monte Carlo technique to account for a "surprising" user patterns for gas appliances, which are reflected in NO_2 emission rates and personal exposures. (People spend very little time standing at a gas range.) Dr. Grot mentioned that the Twin River data may be useful for comparing the user pattern.

Dr. Matthews or ORNL talked about his emission rate model for formaldehyde as a function of room temperature, humidity and room concentration that includes the effect of a permeation barrier. This model has been established using test cell data. He also used the model for field validation of ORNL's unoccupied house data and obtained good agreements. The model assumes that the formaldehyde transfer between a material and the room air obeys Fick's diffusion laws and is time independent.

Mr. Janssen of Honeywell is working on a ventilation efficiency model using recirculation rate and short circuit factor of room supply air. These two factors can be related to the Kusuda mixing factor and Sundberg's ventilation efficiency factor reported previously. He is currently conducting ventilation control experiments using the CO_2 control in a test house under a Bonneville Power Administration contract. A small Japanese-made CO_2 sensor is used to activate an outdoor air damper when the CO_2 level exceeds the set point. He is also testing a simple exhaust fan control scheme using indoor-outdoor temperature difference and wind speed as sensors. The latter has the possibility of being very cost effective. Dr. Moschandreas commented that Janssen's research is appropriate for non-residential buildings where the mixing of supply air is critical. For the residential application, however, he found that the mixing factor is near unity as long as one is addressing the long time phenomena. Mr. Janssen asserted that even for the steady state imperfect mixing occurs. Dr. Mage is interested in residential applications where the short time mixing is important.

Dr. Grot of NBS talked about his current formaldehyde measurement research for CPSC to validate Matthews' ORNL model. His measured data is getting good agreements with a single cell model using the ORNL emission model.

Dr. Mage mentioned the need for the model to include simulation of the effect of air velocity in addition to temperature and humidity, citing an example that the use of a heat exchanger may create drafts undesirable for thermal comfort. Janssen concurred that an air-to-air heat exchanger used at the Bonneville Power Administration test building did produce undesirable drafts as well as noise.

Dr. Ryan of the Harvard School of Public Health talked about the exposure assessment program of a GRI contract research at Harvard and epidemological studies developing the human exposure data needed for this model. He has a microcomputer program for the model developed for two compartments based upon the mass balance principle. For some pollutants he uses empirical data relating the indoor concentration of pollutant to outdoor concentration in relation to air infiltration and emission rate. He also used a Monte Carlo type analysis for simulating the usage pattern of doors between compartments.

Dr. Nagda of Geomet showed his mass balance model that includes, among other things, mixing factor and decay rate. The mixing factor was determined by comparing the measured concentration of CO with the predicted values based upon the air infiltration data obtained from the SF_6 decay method. He found that the mixing factor is usually around unity when the gas range exhaust fan is not in use. It is approximately 10 when the range fan is in operation indicating a strong localized removal of the contaminant. Using this mixing factor he was able to obtain a good agreement between calculated and observed concentrations of CO. His current research is with multizone modeling and stratification, the effects of sources and NO_2 decay rate.

Dr. Davidson of Carnegie-Mellon University is testing three experimental homes whose air leakage rates vary from 2 h^{-1} to 0.1 h^{-1}. Emission rates from stoves and gas driers are measured. Intercompartmental air movement is also measured. Single compartment and multi-compartment models were developed and compared with experimental results. Agreement between test results and models depended upon the type of weather. Agreement was good when the mixing factor was near unity and became worse when mixing factors became different from unity. The worst agreement occurred when mixing was poor. Temperature and humidity had a large influence on NO_2 decay rate. When stoves were turned off, NO_2 decayed rapidly. The decay was assumed to be caused by surface absorption, because the infiltration rate showed only a small effect on decay. He attempted to find re-emission phenomena by observing the NO_2 decay curve, which is expected to deviate from the simple exponential decay if there is re-emission. He was unable to find the re-emission which was similar to the experiences of Moschandreas and Ryan.

Mr. Walton of NBS presented time profiles of contaminant concentration calculated by his multi-compartment Thermal Analysis Research Program (TARP) model. He showed the increase and decay of contaminant concentration in various rooms in a house when the contaminant generation was suddenly started in the kitchen, continued with a constant rate for a while and abruptly turned off. Although the concentration levels are very different among the rooms during the emission stage, the curves for the different rooms seem to merge rapidly as soon as the source was turned off. Grimsrud and Nagda indicated that they observed similar phenomena in their test houses.

Dr. Persily of NBS briefly talked about his work on air leakage measurements for large buildings, indicating its strong dependence on outdoor temperature mainly because of ventilation control schemes employed by building mechanical systems.

Dr. Grimsrud of LBL discussed LBL activities on radon measurements and modeling. He indicated that radon levels varied by a factor of ten even when environmental conditions and air change rates were identical and concluded that radon concentration is source-dominated rather than the air leakage controlled. His associates at LBL developed a model to determine radon migration through soils and are studying the mechanisms of the radon entry into buildings by a pressure balance principle. He then talked about experimental measurements of radon at sump pumps located in basements. Water levels in the sump showed a strong correlation with house radon levels because the high water level in the sump effectively eliminated soil emission. He showed an interesting graph depicting lack of correlation of measured radon levels with infiltration rates. The experimental trend can better be explained if the pressure-induced flow is assumed such that the radon emission rate is proportional to the air infiltration rate, which is a function of pressure difference between in and outdoors. This pressure-driven flow concept could also explain the results reported by others. He indicated that radon levels in soil were near 1000 Pc/L while in the air around the sump they were 500 Pc/L. The pressure differential that is considered to influence the radon entry was in the neighborhood of 3.5 Pa.

The meeting was concluded using a list of parameters, contaminants and the algorithms to be used in the model. After much discussion it was concluded that the parameters to be used in a comprehensive IAQ model are:

- Forced ventilation
- Infiltration (uncontrolled leakage)
- Natural ventilation (through purposeful openings, such as windows)
- Micro-air movement within a space (including movement around a point contaminant source such as a gas range). In this case, the ability to model in small enough time units and grid sizes needs serious consideration.
- Another important element of the micro-movement is the ability to handle ventilation efficacy (defined as the ability of the ventilation to mix, or remove at the source, the contaminants).
- Micro-air movement (room-to-room) (both horizontal and vertical compartments should be included).
- Building architectural descriptions as they affect pollutants
  - Geometry, openings, etc.

- Exposures to the weather.
- Ground contact.

o Weather conditions
  - Outdoor micro-climate (effects of local pollution, temperature, wind, etc.) effected by landscaping, etc.
  - Correlation with weather bureau data.

o Indoor environment (temperature, humidity and other comfort variables).

o HVAC systems, including humidifiers and dehumifiers as they affect pollution levels.

o Pollution removal mechanisms (other than dilution, ventilation).
  - Air treatment devices - point sinks, area sinks.
  - Settling, deposition, absorption, re-emission and pollution capacity of certain materials.

o Sources
  - People, machines and people's activities.
  - Building materials.
  - Consumer products.
  - Outdoor air.
  - Water supply

o Source strength variations - time, temperature, RH, etc.
  - Point sources.
  - Area sources.
  - Effects permeation barriers.
  - Volume source (as in radon daughters).

The most important pollutants to be treated by the IAQ model and the available algorithms should be:

o Radon
  - Source strength (temperature and pressure) (no algorithm exists).
  - Decay and daughter formation (algorithm can be worked out).
  - Daughter removal and decay (Jonnason has algorithms) (attached and unattached daughters).
  - Distribution in spaces (ventilation algorithms needed).

o Formaldehyde
  - Source strength (area, temperature, humidity, space, concentration, time history, material conditioning) (algorithms are well along).
  - Distribition in the space.
  - Decay, absorption, desorption (models not yet developed).
  - Water as a sink (needs modelling).

o NO_2 and NO
  - Source strength (usage pattern and activities) (models well along).
  - Distribution in space.
  - Decay and chemical reaction (model needed).

- Tobacco smoke (sidestream only)
  - Source strengths (models need more work on gaseous constituants).
  - Decay mechanism (better model needed).
  - Distribution in space.

- Particulates (other than tobacco smoke, includes biomaterials and allergens).
  - Source strengths (models needed).
  - Decay, agglomeration, settling, deposition, chemical reactions, size and shape of resuspension (some models exist, more are needed).
  - Distribution in the space.
  - Outdoor sources, geographical location (some models exist).

- CO_2
  - Source strengths (people, combustion) (good models exist).
  - Distribution in space.
  - Absorption and desorption (some models exist).

- CO
  - Source strength (good models exist).
  - Distribution in space (good models exist).

- H_2O (not a pollutant, but its effects on pollutants needs consideration) (H_2O models are good, but the effects on pollutants are not well modelled).

The following pollutants were considered to be important, but could not be modelled with current knowledge, due to the complexity and number of individual pollutants.

- Volatile Organic Compounds (VOC) (other than tobacco smoke).
  - Source strengths.
  - Distribution in space.
  - Decay, absorption and chemical reactions.
  - Human activity and consumer products.
  - Architectural materials.

- SO_2
  - Source strengths (combustion of impure kerosene, coal and wood).
  - Distribution in space.

- Pesticides
  - Source strengths (no models).
  - Distribution in space.
  - Removal (cleaning, mopping, etc.).

The following pollutants were not to be considered, since they are too complex, and no models exist, even though some are important.

- Asbestos (is being handled as a separate problem).

- Micro-organisms and allergens.

- Ozone

Dr. Moschandreas questioned the value of multi-nodal models contending that his model is based on the single node analysis and appears to be adequate. Mage again stressed the importance of multi-nodal models that account for stratification and local high concentration of contaminants occuring in short time intervals.

Dr. Matthew asked; "Are we developing a model applicable to all the pollutants or different models for different pollutants?" Certain pollutants do not require a complex model, while others do. He suggested a series of models for different mechanisms, such as source models, ventilation models, mixing models and feedback models. Responding to Silberstein's question, Matthew explained a fact that the emission rate of a contaminant may be dependent upon its own concentration and he was assured that the feedback is usually included in the general mass balance model.

Responding to Nagda's question on the floor-to-floor migration calculation, Walton indicated that the TARP model already includes that. Mage stressed the importance of micro environmental models to be able to simulate the performance of small personal monitor; where readings at the breathing zone may be dependent upon the size and shape of the wearers.

Other points raised during the discussion were:

1. Absorption and re-emission should be time dependent functions.

2. Pollutant storage in the sources and air should be considered.

3. The radon model requires different treatments for attached and unattached fractions.

Dr. Moschandreas cited a recent paper by Jonnesson dealing with this subject.

It is difficult to measure the source strength of radon and no good model exists to determine the source strength, although the models are sufficiently good for simulating radon decay and daughter formation.

Radon emission rate from water is well known according to Grimsrud. David Harrje of Princeton University is believed to have good data on this subject.

4. Is the Fick's law adequate for permeation barrier models?

5. Is the measurement accuracy good enough to see the effects of air speed over the contaminant emitting surface?

6. Effect of conditioning specimens ... the past history of building products containing formaldehyde as well as the temperature and humidity affect their present source emission rate.

7. Volatile organic compounds (VOC) need categorization because there are so many of them involved. They are generated by various household activities, such as cleaning, hair spraying and furniture polishing.

Yet we know little about any of these contaminants; some are very transitory some vary with occupants' activities, some are internally generated. A suggested classification is to categorize them by whether or not they are due to combustion. Measurements for combustion-based contaminants showed emission rates to vary by a factor of 2 even under supposedly similar conditions.

Outside contaminants from automobile exhaust and gasoline spills originating in attached garages were mentioned as a potential problem.

8. Tobacco smoke: Although it is believed that we know much about the source strength of tobacco smoke, its gaseous source characteristics are not well understood. It is believed to contain over 2000 compounds including formaldehyde (later someone mentioned over 30,000 compounds referring to a National Cancer Institute study). If five measurements were taken, five different answers would result.

   The modellers are interested in the passive smoking aspects. Moschandreas is conducting a passive smoking study. His study revealed that smokers indicated that they smoked fewer cigarettes than they actually did by count, while non-smokers indicated more were smoked than actual.

9. Mulligan mentioned that some contaminants sources are interactive. Some are source-specific contaminants and some sources are connected to many other contaminants.

10. Particulate sources are not well defined: There are many factors to be considered, such as outdoor sources, vacuum cleaners, humidity effects, air motion, solid surface friction, and geographic elements.

11. When considering CO_2 emission, oxygen depletion becomes important for unvented combustion appliances in a small enclosure.

12. CO is a "beautiful" pollutant to study, because it is easy to measure and non-reacting.

A list of recent publications handed out follows.

LIST OF PUBLICATIONS

"Estimated Distributions of Personal Exposure to Respirable Particles", by Richard Letz, P. Barry Ryan, and John D. Spengler. Department of Environmental Science and Physiology, Harvard School of Public Health.

"The Effects of Kerosene Heaters on Indoor Pollutant Concentrations: A Monitoring and Modeling Study," by P. Barry Ryan, John D. Spengler and Richard Letz.

"A Computer Algorithm for Estimating Infiltration and Inter-Room Air Flows," by George N. Walton.

"Formaldehyde Emissions from Combustion Sources and Solid Formaldehyde Resin Containing Products: Potential Impact on Indoor Formaldehyde Concentrations and Possible Corrective Measure," by T. G. Matthews, T. J. Reed, B. J. Tromberg, C. R. Daffron, and A. R. Hawthorne. Sponsored by CPSC. Preprint: Proceedings of the ASHRAE Symposium, "Management of Atmospheres in Tightly Enclosed Space," Santa Barbara, 10/83.

"Ventilation Stratification and Air Mixing," by John E. Janssen, Honeywell, Inc., St. Paul, MN, USA.

"Environmental Dependence of Formaldehyde Emissions from Pressed Wood Products: Experimental Studies and Modeling," by T. F. Matthews, T. J. Reed, C. R. Daffron, and A. R. Hawthorne, Measurement Applications Group, Health and Safety Research Division, Oak Ridge National Laboratory. Sponsored by CPSC. Proceedings: 18th International Washington State University, Particleboard/Composite Materials Symposium.

"Radon Transport Into a Single-Family House with a Basement," by W. W. Nararoff, H. Feustel, A. V. Nero, K. L. Revzan, D. T. Grimsrud, M. A. Essling, and R. E. Toohey. To be submitted to Atmospheric Environment January 1984.

Geomet Report Number ERF-1461, August 1984, "Energy Use, Infiltration, and Indoor Air quality in Tight, Well-Insulated Residences", by Niren L. Nagda, Ph.D., Michael D. Koontz, M.S., and Harry E. Rector, B.S. Prepared for Energy Analysis and Environment Division and Energy Management and Utilization Division, Electric Power Research Institute, Inc.

Attendance Record for the Meeting on IAQ Modeling
February 11, 1985

Room B221 of Building 226
National Bureau of Standards

Cliff Davidson	Dept. of Civil Engineering Carnegie-Mellon University Pittsburgh, PA 15213	412-578-2951
David Grimsrud	Lawrence Berkeley Labartory 90/058 Berkeley, CA 94720	415-486-6591
Richard Grot	National Bureau of Standards Building 226, Room B114 Gaithersburg, MD 20899	301-921-3501
John Janssen	Honeywell, Inc., TSC 1700 W. Highway 36 St. Paul, MN 55113	612-638-5985
James J. Keenan	CPC ESES Washington, DC 20207	301-492-6508
Tamami Kusuda	National Bureau of Standards Building 226, Room B218 Gaithersburg, MD 20899	301-921-3637
Brian Leaderer*	John B. Pierce Foundation 290 Congress Avenue New Haven, CT 06519	203-562-9901
David Mage	U.S. EPA EMSL/RTP MAD/MD-56	919-541-3184
Thomas Matthews	Oak Ridge National Laboratory Building 4500 South Oak Ridge, TN 37831	615-574-6248
P. E. McNall	National Bureau of Standards Building 226, Room B226 Gaithersburg, MD 20899	301-921-3447
D. J. Moschandreas	IIT Research Institute Chicago, IL 60616	312-567-4310
J. L. Mulligan	CPSC ESES Washington, DC 20204	301-492=6508
Niren Nagda	Geomet 20251 Century Blvd. Germantown, MD 20874	301-428-9898

Andrew Persily	National Bureau of Standards Building 226, Room B114 Gaithersburg, MD 20899	301-921-2330
P. Barry Ryan	Harvard School of Public Health 677 Huntington Avenue Boston, MA 02115	617-732-1431
Samuel Silberstein	National Bureau of Standards Building 226, Room B114 Gaithersburg, MD 20899	301-921-2758
Kevin Teichman	Dept. of Energy Washington, DC	202-252-9187
George Walton	National Bureau of Standards Building 226, Room B114 Gaithersburg, MD 20899	301-921-3633

*Brian Leaderer's inputs were received later in the evening of Febraury 11, due to a travel delay.

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10. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

Comprehensive modeling of emission, absorption, movement and controls of indoor air contaminants is essential for developing national policy for IAQ assessment and controls. This report describes several topics discussed in a workshop on indoor air quality, which was held on February 11, 1985 at the National Bureau of Standards. Researchers on IAQ modeling were invited to state their current activities, identify future research needs and recommend specific parameters and contaminants to be included in the IAQ models. The input thus obtained in this workshop will be incorporated in an advanced simulation model for IAQ, to be developed by NBS under a contract with EPA.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

absorption; air circulation; contaminants; emission; indoor air quality; simulation models

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