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Standard Guide for Statistical Evaluation of Indoor Air Quality Models[1]

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1. Scope

1.1 This guide provides quantitative and qualitative tools for evaluation of indoor air quality (IAQ) models. These tools include methods for assessing overall model performance as well as identifying specific areas of deficiency. Guidance is also provided in choosing data sets for model evaluation and in applying and interpreting the evaluation tools. The focus of the guide is on end results (that is, the accuracy of indoor concentrations predicted by a model), rather than operational details such as the ease of model implementation or the time required for model calculations to be performed.

1.2 Although IAQ models have been used for some time, there is little guidance in the technical literature on the evaluation of such models. Evaluation principles and tools in this guide are drawn from past efforts related to outdoor air quality or meteorological models, which have objectives similar to those for IAQ models and a history of evaluation literature (**1**).[2] Some limited experience exists in the use of these tools for evaluation of IAQ models.

1.3 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.4 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[3]

D1356 Terminology Relating to Sampling and Analysis of Atmospheres

3. Terminology

3.1 *Definitions*—For definitions of terms used in this standard, refer to Terminology D1356.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *IAQ model, n*—an equation, algorithm, or series of equations/algorithms used to calculate average or time-varying pollutant concentrations in one or more indoor chambers for a specific situation.

3.2.2 *model chamber, n*—an indoor airspace of defined volume used in model calculations; IAQ models can be specified for a single chamber or for multiple, interconnected chambers.

3.2.3 *model evaluation, n*—a series of steps through which a model developer or user assesses a model's performance for selected situations.

3.2.4 *model parameter, n*—a mathematical term in an IAQ model that must be estimated by the model developer or user before model calculations can be performed.

3.2.5 *model residual, n*—the difference between an indoor concentration predicted by an IAQ model and a representative measurement of the indoor concentration; the value should be stated as positive or negative.

3.2.6 *model validation, n*—a series of evaluations undertaken by an agency or organization to provide a basis for endorsing a specific model (or models) for a specific application (or applications).

3.2.7 *observed model bias, n*—a systematic difference between model predictions and measured indoor concentrations indicated by model residual (for example, the model prediction is generally higher than the measured concentration for a specific situation).

3.2.8 *pollutant concentration, n*—the extent of the occurrence of a pollutant or the parameters describing a pollutant in a defined airspace, expressed in units characteristic to the pollutant (for example, mg/m^3, ppm, Bq/m^3, $area/m^3$, or colony forming units per cubic metre).

4. Significance and Use

4.1 Using the tools described in this guide, an individual seeking to apply an IAQ model should be able to (*1*) assess the performance of the model for a specific situation or (*2*) recognize or assess its advantages and limitations.

[1] This guide is under the jurisdiction of ASTM Committee D22 on Air Quality and is the direct responsibility of Subcommittee D22.05 on Indoor Air.

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[2] The boldface numbers in parentheses refer to the list of references at the end of this standard.

[3] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

4.2 This guide can also be used for identifying specific areas of model deficiency that require further development or refinement.

5. Components of Model Evaluation

5.1 The components of model evaluation include the following: (*1*) stating the purpose(s) or objective(s) of the evaluation, (*2*) acquiring a basic understanding of the specification and underlying principles or assumptions, (*3*) selecting data sets as inputs to the evaluation process, and (*4*) selecting and using appropriate tools for assessing model performance. Just as model evaluation has multiple components, model validation consists of one or more evaluations. However, model validation is beyond the scope of this document.

5.1.1 *Establishing Evaluation Objectives:*

5.1.1.1 IAQ models are generally used for the following: (*1*) to help explain the temporal and spatial variations in the occurrences of indoor pollutant concentrations, (*2*) to improve the understanding of major influencing factors or underlying physical/chemical processes, and (*3*) to predict the temporal/spatial variations in indoor concentrations that can be expected to occur in specific types of situations. However, model evaluation relates only to the third type of model use—prediction of indoor concentrations.

5.1.1.2 The most common evaluation objectives are (*1*) to compare the performance of two or more models for a specific situation or set of situations and (*2*) to assess the performance of a specific model for different situations. Secondary objectives include identifying specific areas of model deficiency. Determination of specific objectives will assist in choosing appropriate data sets and quantitative or qualitative tools for model evaluation.

5.1.2 *Understanding the Model(s) to be Evaluated:*

5.1.2.1 Although a model user will not necessarily know or understand all details of a particular model, some fundamental understanding of the underlying principles and concepts is important to the evaluation process. Thus, before evaluating a model, the user should develop some understanding of the basis for the model and its operation. IAQ models can generally be distinguished by their basis, by the range of pollutants they can address, and by the extent of temporal or spatial detail they can accommodate in inputs, calculations, and outputs.

5.1.2.2 Theoretical models are generally based on physical principles such as mass conservation (**2, 3**). That is, a mass balance is maintained to keep track of material entering and leaving a particular airspace. Within this conceptual framework, pollutant concentrations are increased by emissions within the defined volume and by transport from other airspaces, including outdoors. Similarly, concentrations are decreased by transport exiting the airspace, by removal to chemical/physical sinks within the airspace, or for reactive species, by conversion to other forms. Relationships are most often specified through a differential equation quantifying factors related to contaminant gain or loss.

5.1.2.3 Empirical models (**3**) are generally based on approaches such as linear regression analysis, using measurements under different conditions across a variety of structures, at different times within the same structure, or both. Theoretical models will generally be suitable for a wide range of applications, whereas empirical models will generally be applicable only within the range of measurements from which they were developed.

5.1.2.4 Some combination of theoretical and empirical components is also possible. Specific parameters of a theoretical model may have relationships with other factors that can be more easily quantified than the parameters themselves. For example, the rate of air infiltration into a structure could depend on outdoor windspeed and the indoor-outdoor temperature difference, or the emission rate from a cigarette could depend on the combustion rate and the constituents of the particular brand smoked. Given sufficient data, such relationships could be estimated through techniques such as regression analysis.

5.1.2.5 IAQ models may be specified for a particular pollutant or in general terms; this distinction is important, for example, because particle-phase pollutants behave differently from gas-phase pollutants. Particulate matter is subject to coagulation, chemical reaction at surfaces, gravitational settling, diffusional deposition, resuspension and interception, impaction, and diffusional removal by filtration devices; whereas some gaseous pollutants are subject to sorption and, in some cases, desorption processes.

5.1.2.6 Dynamic IAQ models predict time-varying indoor concentrations for time steps that are usually on the order of seconds, minutes, or hours; whereas integrated models predict time-averaged indoor concentrations using average values for each input parameter or averaging these parameters during the course of exercising the model. Models can also differ in the extent of partitioning of the indoor airspace, with the simplest models treating the entire indoor volume as a single chamber or zone assumed to have homogeneous concentrations throughout; more complex models can treat the indoor volume as a series of interconnected chambers, with a mass balance conducted without each chamber and consideration given to communicating airflows among chambers.

5.1.2.7 Generally speaking, as the model complexity grows in terms of temporal detail, number of chambers, and types of parameters that can be used for calculations, the user's task of supplying appropriate inputs becomes increasingly demanding. Thus users must have a basic understanding of the underlying principles, nature and extent of inputs required, inherent limitations, and types of outputs provided so that they can choose a level of model complexity providing an appropriate balance between input effort and output detail.

5.1.2.8 A number of assumptions are usually made when modeling a complex environment such as the indoor airspace. These assumptions, and their potential influence on the modeling results, should be identified in the evaluation process. One method of gaining insights is by performing sensitivity analysis. An example of this technique is to systematically vary the values of one input parameter at a time to determine the effect of each on the modeling results; each parameter should be varied over a reasonable range of values likely to be encountered for the specific situation(s) of interest.