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Workshop on Harmonization of Serving Future Needs with Occupational Exposure Databases—Inhalation Modeling, Session IIIA

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This workshop was one of several that took place at the International Symposium on Occupational Exposure Databases and Their Application for the Next Millennium held in London from November 1–3, 1999. About 30 delegates participated in the workshop. The agenda for the discussions was provided by a white paper prepared by the organizers. The workshop produced a conceptual outline for a general-purpose prediction model for inhalation exposure, and constructed a list of important input variables for successful model development. Evaluation of prototype models was discussed in some detail, and the workshop concluded with suggestions for taking forward the ideas discussed and maintaining the momentum and interest generated during the symposium.

An International Symposium on Occupational Exposure Databases and Their Application for the Next Millennium took place in London from November 1–3, 1999. The symposium was sponsored by the American Conference of Governmental Industrial Hygienists (ACGIH®), in collaboration with the United Kingdom Health and Safety Executive (HSE), the British Institute of Occupational Hygienists (BIOH), the American Industrial Hygiene Association (AIHA) and the European Chemical Industry Council (CEFIC). The symposium programe consisted of a number of technical sessions, in which about 50 formal papers were presented, and several workshops which discussed and developed topics of current interest and concern.

Workshop IIIA was concerned with harmonizing knowledge and opinion on the computer modeling of inhalation exposure. Interest in this topic has increased in recent years, because of:

1. a need to be able to predict exposures to new substances before they are put on the market and
2. the escalating costs of gathering measured data and the limited availability of qualified people to undertake this work.

The scene was set by a white paper (Annex I) prepared by the workshop organizers. Taking this as their agenda, the delegates participating in the workshop discussed many aspects of computer modeling in detail. This report summarizes those discussions and makes some suggestions for maintaining international communication and stimulating future development in this important area.

CHARGE TO THE GROUP

The workshop delegates received the following charges:

1. Identify the critical data needs and approaches that will enable occupational hygienists in the 21st century to develop, validate, and use appropriate predictive models for evaluating and managing occupational exposures.
2. Develop recommendations for promoting via an international forum, the continued development, validation, and use of these approaches.

Report

About 30 delegates attended the workshop sessions, and most of them took an active part in the discussion. In the first session on Tuesday, the group explored the entire subject of inhalation modeling with the aim of establishing the range of views, based on the individual's own perceptions and experience. Discussion covered the basic needs for models (e.g., should a model be used as a screening tool or as an exposure predictor?), what models should be able to do, and what types of models would meet these stated aims. In addition, it was recognized that models would need to be closely linked to databases both for development and validation purposes. It was generally considered that models should be simple in concept, and might need to have some standardized properties (e.g., the ability to predict exposure as a probable range of airborne contaminant concentrations).

There was considerable discussion on the relative merits of mathematical and knowledge-based models, which converged on a concept in which a central core model, which might be either logical or deterministic in form, could call up a range of specific process models built to deal with particular circumstances (e.g., paint spraying) in detail. This concept is illustrated in Figure 1. In the conceptual model, the core module takes input data on the process, substance, work activity, etc. and generates a predicted or estimated range of inhalation exposure to the substance of interest. This process can either make use of measured exposure data held in the model software itself, or call up predetermined exposure ranges derived from a comprehensive occupational exposure database. For some well-defined processes, such as paint-spraying in booths or drum filling and opening, it may be possible to design mathematical models based on computational fluid dynamics or the results of specific research projects. Where such models provide more reliable and accurate estimates of exposure, the core module will call them up when the input parameters suggest that they are suitable.

The model will need to operate both retrospectively and prospectively, i.e. it will be able to estimate exposure to existing substances in current or historical use and also to predict exposure to new substances and for novel processes. This will be done by analogy with experience, for example by matching the vapour pressures of solvents. The available evidence is that exposure for new substances can be predicted with an acceptable degree of reliability in these circumstances.

Finally, a full description of the model will be openly available. This type of modelling is evolutionary in nature and its precision will improve if it is able to keep pace with the development of knowledge and the accumulation of experience. Consequently, the model will be accompanied by detailed information on the assumptions employed in its development, the methodologies used in its construction and the extent of the uncertainty associated with its outputs. Once it is developed, the model will need to be validated against independent measured exposure data and subsequently modified in the light of this validation exercise. This is seen as a continuing activity, which will make sure that the model both maintains its currency and improves with time. There was general agreement that this idea would work well as a general concept.

With this background in mind, and using some of the ideas in the white paper, the second session on Wednesday considered what data should inform model development and what variables were important. In general, the model should contain parameters representing the source of exposure, the exposure "receptor" (representing various factors such as the use of personal protective equipment (PPE) and behavioral influences which will affect exposure), and the transport of the exposure from the source to the receptor. Variables were grouped into several categories, including:

1. Type of work process
   - manual operation, automatic or other
   - continuous, batch, or other process
     - indoor versus outdoor—details on ventilation
     - personnel (stationary or mobile).

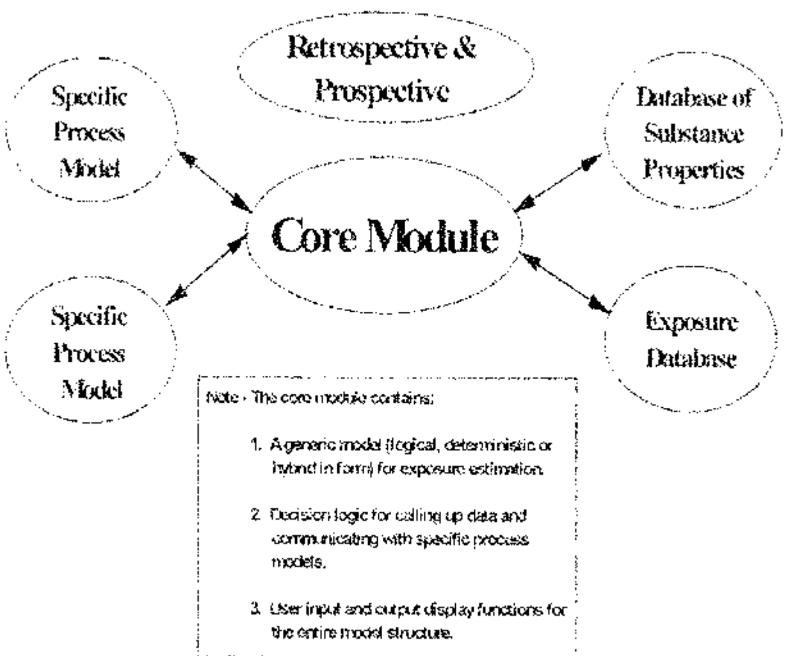

FIGURE 1
Idealised framework for a predictive exposure model.

2. Library of chemical/physical properties—complete and validated information.
3. Quantity and properties of materials—define source properties and generation rate characteristics.
4. Descriptions of exposure control systems, the use of personal protective equipment, and their effectiveness—containment, ventilation, or other controls.
5. Behavioral and work practice descriptors
   - activity duration, frequency tied to exposed activities.
6. Survey strategy and survey objectives.
7. Recording/analysis of direct reading (data logging) information for database and model development, etc.
8. Workplace conditions/patterns of exposure
   - routine operations
   - upper-end or worst-case conditions.
9. Nature of health endpoint
   - acute versus chronic
   - temporary and reversible versus permanent and disabling.
10. Data needs for development and evaluation versus data needs for model use.

As well as details of the work process, and job description, elements relating to properties (including source generation terms) of the contaminant substances were considered important, and it was felt that an a standardised and validated electronic database of substance properties would be essential. Information would also be required on source properties and contamination generation rates.

Control systems and their effectiveness, and behavioral characteristics should also be included. Where actual measured data are used for developing the model, there should be good information on the quality of the data and the purposes for which it was collected (e.g., random survey, compliance data, substance survey, etc.), to provide information on whether it is was typical or worst-case information. Data obtained by "non-traditional" means (e.g., direct-reading instruments and data loggers) should be mentioned, as well as workplace conditions. Some consideration would also need to be given to health endpoints (acute/chronic) and the employment of safety factors for substances/circumstances of which the health endpoints are uncertain. It would be necessary to maintain a source of independent data, not used for model development, for testing and validating prototype models.

Model evaluation, if done comprehensively, is a complex process involving the following elements:

1. Assessment of software operation (logical structure, quality assurance).
2. Testing of the model algorithms and their robustness, accuracy and limits.
3. Relevance and accuracy of the model—also whether its outputs are useful and comprehensible.
4. Comparison of model outputs/predictions with a consensus of informed professional judgment.
5. Comparison with measured data from analogous situations.

Each of these elements should be considered at the project planning stage, and built in to the project management process. In particular, software testing and assurance should be undertaken by an independent IT specialist who can apply the rigorous procedures needed to make sure that the software contains no internal inconsistencies and meets its design specification. For the overall project, all development stages and records should be recorded and easily traceable. At every stage, the model development should proceed by consultation, to achieve a consensus model which will ultimately have the endorsement and confidence of the professional community as a whole.

THE WAY FORWARD

The group recognized that none of this would be achievable without a great deal of discussion and consultation on an international basis. With modern technology (especially e-mail and the Internet) this is not an insurmountable problem, but it does require effort and application. Means of keeping in touch suggested by group members included:

1. Active participation in newsletters.
2. Promotion of papers and sessions on modeling at future conferences and symposiums.
3. Participation in the work of appropriate committees of professional institutions and associations.
4. More extensive use of the Internet and list serves, although the last item should be used with caution, as several members of the group reported problems with the proliferation of trivial messages and the use of list serves for commercial marketing purposes.

In addition, the group felt quite strongly that there should be a more formalized arrangement with governmental committees, standards committees, and so on setting up working groups to develop models and their philosophy. The groups should have representation from government, academia, labor, and industry to achieve maximum effectiveness. It was not considered that the group had any direct influence over setting up these arrangements, but this report might be used to stimulate either an existing committee of ACGIH, BIOH, or other professional bodies in North America and Europe to take this topic forward, or to set up a new committee/subcommittee to do so.

Annex I
White Paper—Workshop IIIa
Harmonisation of Future Needs—Inhalation Modeling

CHARGE TO THE GROUP

1. Identify the critical data needs and approaches that will enable occupational hygienists in the 21st century to develop,

validate, and use appropriate predictive models for evaluating and managing occupational exposures.
2. Develop recommendations for promoting via an international forum, the continued development, validation, and use of these approaches.

BACKGROUND

As we look to the future of occupational exposure assessment, two issues of immediate importance can be identified. One is the important role of the use of predictive modeling techniques to be used in the absence of acceptable monitoring data, and the second is the importance of dermal exposure on the overall body burden. Both of these issues are in need of additional research to enable us to readily employ these approaches, but more importantly, both may require us to collect additional or different information to support their continued development and use.

Modeling techniques are commonly used throughout the United States and in Europe. Other countries are also using predictive approaches. Many United States models are based on empirical or theoretical approaches, while some of the models used in Europe are based on logic models. In practice it is not uncommon to combine both approaches to assess occupational exposures.

This white paper presents some thoughts on the topics of exposure prediction modeling approaches and dermal exposure assessment with a goal towards stimulating discussion on what needs to be accomplished if we are to be able to use models in the future for assessing exposures, and to better understand and manage dermal exposure.

INHALATION EXPOSURE PREDICTION MODELS

Exposure can be predicted by a variety of means. In some ways any statement about exposure is a prediction; even measurements are predictions in the sense that they provide an estimate of the true concentration (which is unknowable), and many assumptions are made in saying that a measurement represents an actual exposure.

A. Review of Approaches

With this idea in mind let us look at what we are trying to do. There is an undoubted need for some form of assessment tool that says "From the information that we have, the best available knowledge says that exposure in these circumstances is likely to be about XXX." If we can look at all the factors which influence exposure, then we can fabricate a model that predicts XXX as reliably as our knowledge allows. Possible conceptual approaches are:

1. Personal estimation from past experience (relies on knowing the results of past measurement and on occupational hygiene expertise).
2. Application of a mechanistic model, i.e. a model developed from considerations of classical physics/chemistry/engineering theory, which calculates an estimate based on fundamental principles and the properties of the substance.
3. Application of a knowledge-based model which compares the circumstances under consideration with similar circumstances in a hierarchy of knowledge, and provides an estimate based on past measurements of exposure under similar circumstances.

What we are concerned with are items 2 and 3. They represent two different approaches to modeling—the deterministic models, and the empirical/decision tree type models. They each have their uses, strengths, and weaknesses, and rely on the accuracy of input information for their performance. As it happens, the current position (1999) is that deterministic models appear to be favored in North America, while in Europe a model based on an expert system has been in use for several years. A combined approach is also possible. For example, pesticide models as used in registration are sometimes a mixture of the two, with logical separation of different scenarios based on knowledge, and calculations for specific scenarios based on part theory and mostly knowledge. However, it is true that some models are close to calculations based on primary physicochemical parameters and others close to logical decision trees. Therefore, such a division is useful. Neither of the approaches is intrinsically superior to the other: each has its limitations and advantages, some examples of which are presented in Table I:

As models are always tentative in nature, and the two types are created in very different conceptual environments, there is something of a tendency for them to diverge as they develop. Deterministic modelers will want to extend the precision of their equations and make use of additional factors (e.g., incorporating detailed properties of ventilation sources and creating complex matrices for calculating theoretical air velocities and distributions). This can lead, for example, to multidimensional spatial plots of contaminant concentration which will need to be integrated over time and space to estimate an exposure profile. Conversely, knowledge-based systems may well tend to a greater degree of generality, which will produce estimations in the form of a range of expected exposures, possibly associated with some form of probability of occurrence.

B. Basic Data Needs

The two approaches have differing requirements for the basic information which they use for determining their predictions. The following lists indicate the type of basic information that is needed for each. It is emphasised that the lists are informative only and are not intended to be exhaustive. It is also true that future models may incorporate features of both the deterministic and the knowledge-based approaches. The two types are not mutually exclusive.

1. Deterministic Models

Source. Evaporation or spray rate; quantity of substance present and/or usage rate; estimation of dust generation rate; composition of source(s); air and liquid temperature(s); qualitative description of process; controls in place; physical/chemical properties of the substance.

TABLE I

Pros	Cons
1. Deterministic models	
Rigorous, based on logical argument and developed from sound principles	Applicable to a limited range of theoretical circumstances—cannot be extended to (new) situations with insufficient knowledge of the circumstances
Can be developed as computer software, with powerful computational potential	No allowance for practical deviations from classical theory
Fast output, as precise as desired	Different models needed for different processes and types of substance. Can result in false accuracy of exposure estimated
	Different models needed for different processes and types of substance
Output can be plotted as time history or as spatial variation	May need specialized knowledge for successful operation and interpretation
Can be modified and improved over time	Need for validation by comparison with independent data
Can evaluate uncertainty and sensitivity using quantitative approaches (e.g., Monte Carlo analysis)	May need substantial computer memory for operation
	Need to know the generation rate, which can be very difficult to model
	Generally assess concentrations in a space at a time or the distribution of concentrations in space and time and not (average) exposure levels
	The need to know where (compared to a source) a worker is when (compared to an activity or process) makes estimation of personal exposures by concentration models very difficult
	Sometimes need to know input parameters whose values are not easily available
2. Knowledge-based models	
Applicable to a wide range of circumstances, and can be extrapolated	No calculation—output specified as a range of likely exposures
Based on a large corpus of knowledge and experience	Considerable interpretation necessary at both input and results stages
Can be refined and adapted to cover new scenarios and circumstances	Dependent on accuracy and reliability of input data
Based on a large body of measured data (therefore related to real life)	Based on a large body of measured data (can be cumbersome to modify/develop)
Results can be modified to account for factors not considered by the model	Need for validation by comparison with independent data
Can be developed as expert-system software	Results can be misinterpreted
	Can only be developed when sufficient relevant knowledge is available

Time Course. Activities list with details of: When and how long the various activities occurred during the sampling.

Sinks. A determination and matching of the kinetic coefficients of adsorption, desorption, and degradation to the surfaces in the workplace. A listing of the various surfaces and their surface areas in the monitored area.

Ventilation and Dispersion. On-site determination of air exchange rate; eddy diffusivity, directionality, and velocity of air movement at the monitoring location. Measured room dimensions. Type of structure from a checklist of possible types.

Techniques. Computational fluid dynamics; mass balance; thermodynamics/physical chemistry; use of empirically derived relationships.

2. *Knowledge-Based Models*

Substance. Physical properties (gas/liquid/vapor), estimation of tendency to become airborne (may also include information on the quantity of substance used or usage rate).

Categories of Use/Process. Spectrum of categories, ranging from totally enclosed processes to widely dispersive use in uncontrolled or poorly ventilated environments; listing of distinct (main) process types with major differences in exposure.

Categories of Control. Local exhaust ventilation, dilution ventilation, control by segregation, substance modification (e.g., pelletizing dusty solids, etc.).

Techniques. Application of experience, preexisting knowledge, inference, and analogy to predict likely exposure based on similarity of physical conditions and behavior patterns. Statistical data analysis. Data are combined into more or less homogeneous groups to optimize the statistical significance of the output.

C. Future Needs for Inhalation Exposure Prediction Models

Models tend to be developed by individuals, who will make use of a variety of source information (published literature, personal experience, cross-fertilization with colleagues, etc.). However, for any model to achieve broad acceptability across the occupational hygiene community (nationally, internationally, and between continents), it must be:

1. transparent in its derivation and construction
2. widely discussed and validated, and effectively peer-reviewed
3. open to further development and validation over time.

Consequently, there must be opportunities for the model to be tested in a wide variety of circumstances and modified in the light of the results of these tests. This implies access to a lot of different data sources, and an openness of approach for analyzing test results and modifying the model design. This also highlights a substantial opportunity for sharing and leveraging knowledge and resources to most effectively utilise our collective expertise.

These are issues for which confidence needs to be built up over time. One fruitful approach might be to set up an international (computer-) modeling forum, on either a formal or an informal basis, to take this subject area forward.