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GOOD MANUFACTURING PRACTICE FOR MODELLING AIR POLLUTION: QUALITY CRITERIA FOR COMPUTER MODELS TO CALCULATE AIR POLLUTION

C. M. DEKKER
Quality Control Information Systems Ltd, Archimedesbaan 13, 3439 ME Nieuwegein, The Netherlands

and

C. J. SLIGGERS
Ministry of Housing, Physical Planning and Environment, Air Directorate, P.O. Box 450, 2260 MB Leidschendam, The Netherlands

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Abstract—To spur on quality assurance for models that calculate air pollution, quality criteria for such models have been formulated. By satisfying these criteria the developers of these models and producers of the software packages in this field can assure and account for the quality of their products. In this way critics and users of such (computer) models can gain a clear understanding of the quality of the model. Quality criteria have been formulated for the development of mathematical models, for their programming—including user-friendliness, and for the after-sales service, which is part of the distribution of such software packages. The criteria have been introduced into national and international frameworks to obtain standardization.

Key word index: Quality assurance (computer) models, quality criteria, mathematical models, software, user-friendliness, after-sales service.

INTRODUCTION

The use of mathematical models to determine air pollution is growing steadily. It is nearly always cheaper to use mathematical models than to carry out extensive measurements. Moreover, it is impossible to carry out measurements for each place at which the quality of the air has to be determined. Carrying out some measurements, such as those for future situations and scenario studies, is often even impossible. These considerations have led to the situation that for controlling air quality and maintaining limit-values, in some cases, calculations and measurements are made equal before the law in The Netherlands. Demands are made upon the outcomes of calculations with regard to reliability and accuracy. In The Netherlands, mathematical models are also used when making policy decisions on such issues as abating acidification and the greenhouse effect. For these reasons the models themselves and the software packages of such models should meet a verifiable quality. For this reason the Air Directorate of the Ministry of Housing, Physical Planning and Environment investigated how to improve quality with regard to mathematical models and software packages in the field of air pollution. The results of this research have been included in the Publication Series Air (Dekker *et al.*, 1990). In this report criteria have been formulated with regard to the quality of the mathematical model, the quality of the software package and the quality of the after-sales service. Also the way these criteria can be met is dealt with extensively.

The Ministry has dedicated itself to national and international acceptance of these criteria. This article briefly outlines what quality criteria for air-pollution calculation models may look like and how they can be complied with. In the tables, quality criteria are mentioned which are described in greater detail in Dekker *et al.* (1990). In this article most are highlighted.

Lack of quality criteria is not a problem that is confined to models in the field of air pollution. The quality criteria that have been formulated for air pollution can also be used to enforce the quality of other models.

Quality criteria for computer models
Mathematical models
Software packages
User-friendliness
After-sales service

QUALITY CRITERIA

Nowadays a lot of attention is paid to quality assurance for measurements. Laboratories must work under "Good Laboratory" (GLP) and "Good Manufacturing Practice" (GMP) conditions to be able to guarantee quality. In The Netherlands laboratories can be certified by means of a so-called "Starlab" hallmark, if their quality procedures comply with specified GLP- and GMP-requirements. The outcome of the calculations is just as or even more important than the outcome of the measurements. Therefore the development of models, and calculations with the help of models should also fall under GMP- or GLP-requirements. To spur on quality assurance for models in The Netherlands the choice has been made to formulate quality criteria for the GMP of air-pollution models. GLP-guidelines for working with models have been left aside.

The quality criteria are formulated as performance features and not as quantative requirements. In this way the criteria can be general and valid for all models. Developers of models and producers of software packages have to describe the quality of their products. They do so by filling in the quality criteria. In this way the onus of proof of quality of the model and the software package lies with the developers and producers. Critics and users can form their own opinions about the performance of the model, the software package and the service by examining the description of the developers and producers.

When formulating the criteria several conditions have been taken into account. The principle has been adhered to that the model and software package should fit in with the current practice with regard to the development of mathematical models and software packages as much as possible. If they do fit in, this will enable the quality criteria to be accepted sooner. Also, international standards and regulations have been taken into account. As far as these are available, they are interesting, businesswise, for package developers who operate on the international market. Implementation procedures of environmental software packages in an organization and the financial consequences of the formulated quality criteria for existing or future mathematical models and environmental software packages have been left aside.

Quality criteria for mathematical models

Mathematical models are expected to describe reality, so they have to model well and accurately. How well the model describes reality depends on the current state of science, of technology and on financial limitations which will be imposed on the development of mathematical models. That is why premises and limiting conditions are necessary to reduce the complexity of the mathematical model. These premises and limiting conditions are acceptable if the discrepancy between the results from the model and reality is not too large. How much a model deviates, and in which situations the calculations by these models represent a given situation, determine the quality of the model. A developer of models should provide insight into the quality of his model by giving a description of certain aspects. For this description quality criteria have been formulated. By meeting these criteria the developer indicates the quality of the model. He has to explain the operating procedure of the mathematical model on the basis of a flow chart. He also has to include a description of the principles and the mathematical formulae. The scope has to be specified. Aspects of the scope are variations in time and space, type of sources, the desired accuracy of the input, etc. So what the model may be used for is described here. Validation of the model is perhaps the most important aspect of the quality of the model. Aspects of validation are sensitivity analysis, uncertainty analysis and accuracy. The degree in which changes of parameters influence the results of the mathematical model, is called sensitivity analysis. This sensitivity analysis has to be carried out for the input parameters as well as for the internal model parameters and gives an insight into the robustness of the model. Parameters which cause a significant change in the results of the mathematical model deserve extra attention. An uncertainty analysis also belongs to the validation of the model. Assumptions and uncertainties which are at the basis of the model and the choice of the internal model parameters have their influence on the outcome of the model. How much influence they have is the result of this analysis. The output of the model has to be verified with the results from measurements and other validated models. Of course various statistical techniques should be given which show the accuracy of the mathematical model.

Quality criteria for mathematical models
Operating procedure of the model
Scope
List of parameters
Accuracy of input
Parameter variability
Uncertainty analysis
Extreme conditions
Comparison with other models
Comparison with measurements
Traces
Degeneration

Apart from the above-mentioned quality criteria an important way to increase the quality of a model is to use a development method when making a mathematical model. It appeared that most model developers do not manage the development of their model. The development of a mathematical model according to the method of the Environmental Protection Agency (EPA, 1984) can be a guidance to quality. This method splits the developmental process of the mathematical model into: a preliminary investigation in which the emphasis is on the requirements of the scope, the sources and the surrounding of the sources; and a phase for the making of a performance-evaluation protocol that clearly shows in which respect and on which points the mathematical model has to do well to fall within the acceptance requirements. By quantifying concepts like good, better and best as much as possible in the performance-evaluation protocol an attempt is made to quantify the quality of the mathematical model. That is why it is important to plan the performance-evaluation protocol before the first test results are known. Experience shows that the starting points are changed because the test results do not match. After the drawing up of the performance-evaluation protocol and the determination of the data sets which are to be used, the measurements come up. The measurements—which, of course, have been carried out under GLP conditions—are followed by the analysing of these measurements; then the results are compared with the results of the model and finally these data are submitted to the performance-evaluation protocol. In this way the development of a model is structural and the information obtained can be used in filling in the quality criteria.

Quality criteria for software packages

When a mathematical model has been developed, it has become normal practice that such models appear on the market as software packages. Though mathematical models are usually developed with the help of computers, the question is whether the software made by the developers of models is good enough to be applied generally. Mathematical models are usually developed without the specific objective to realize a software package for common use. If the mathematical model works well, the developmental stage is left and then often the switch is made to the realization of a package that is more or less suitable for other users. Usually the developer of a model is hardly concerned about the user-friendliness, the uniformity, the use of programming conventions and the possibility of maintenance. Users do, however, make such demands.

Therefore the development of the software package should take place under the control of a Software Quality Assurance (SQA) plan. How the quality of the developmental process which is to be carried out, and the quality of the products which are to be supplied, is going to be monitored and checked, is indicated in such a plan. The SQA-plan guarantees a software package that has been effected in a balanced way and in which all relevant quality aspects have played their parts. A SQA-plan can be tied to a particular project; that means that the arrangements and procedures are tuned to the project for which the SQA-plan was designed. This leaves great freedom in the degree of detail with which these arrangements and procedures are filled in. However, with regard to some points the SQA-plan must comply with common features: it must always contain the phases and interim reports which are to be delivered, the documentation and the design- and code standards.

Quality criteria for software packages: Software Quality Assurance plan
Description of the project
Phases and interim reports
Planning and control
Organization
Reviews and audits
Proposed changes
Configuration and change management
Documentation
Tests
Tools
Design standards
Code standards

Which development method has been applied must be shown in the phases and interim reports. Should the development method be used in a way that differs from the prescribed way, then this should be indicated. Though the development method "System Requirements Specification" (SDM) is usually used in The Netherlands, the internationally highly regarded and accepted development method of the Institution of Electrical and Electronic Engineers (IEEE, 1984, 1986) is recommended because this guarantees a better compatibility with Dutch software packages on the international markets. These IEEE standards have, although in a slightly different form, already been applied to full satisfaction at the Delft Hydraulics (WL) in The Netherlands (Delft Hydraulics, 1989). Another reason to choose the IEEE standards is the conviction that the producers of environmental software will be in a better position to acquire a standing on the international market where there is an increasing demand for reliable software.

Apart from the Software Quality Assurance Plan an important recommendation is the use of uniformity in computer language. This makes serviceability and maintenance of the developed mathematical models more simple. Also (parts of) the model can be incorporated in other models without any problems. So far Fortran has been the most frequently used computer language for the developing of software packages in the field of air pollution in The Netherlands. The Royal Dutch Metereological Institute (KNMI) developed conventions for Fortran '77 (KNMI, 1987). These conventions contain arrangements like "All factors which are dependent on a machine or operating system must be put in isolated routines" and "Every routine may not exceed the complexity of 600 points, with an executable statement counting as 1 point, calling a subroutine 5 points and every branche 10 points". Strictly speaking no scientifically accepted quality criteria can be given for the size of programs. The choices of the KNMI are mainly based upon practical grounds and should not be applied too rigidly.

Quality criteria for user-friendliness

The first demand that must be made upon software packages is that working with the package should be relatively simple. Moreover, the multitude of packages available causes a great need for uniformity. Common problems for experienced users are use of the function keys, presentation of the error messages and data entry. These should not lead to insurmountable problems but can lead to loss of time and annoyance. That is why a choice has been made to formulate quality criteria in the field of user interfaces. Quality criteria have been formulated, among other things, for help functions, the maintenance of the data, the presentation of the screens and the surveys, the error messages and the protection of the software package against viruses by means of checksum totals.

Quality criteria for user-friendliness
Menus
Release management
Back up and recovery options
Installation of the package
Specification of concepts and definitions
Help functions
Updating, maintenance of data
Starting the application
Screens
Surveys
Error messages
Entry securities
Package securities
Package protection

For screens, quality criteria have been formulated like "Prompts (the hard text or names of fields) are written in small letters with an initial capital letter" and "Abbreviations are not ended with a dot". These may not be such startling quality criteria, but they are quality criteria which lead to uniformity of software packages and that is the goal. For the maintenance of data a link has been made to the Common User Access (CUA) guidelines (IBM, July and Dec. 1989), which are defined within the SAA strategy of IBM and are based on the "object-action" principle (Gebius and Metsaars, 1990). This object-action principle implies that first the object, e.g. article 12345, is chosen and only then the action like change, delete, calculate. Expectations are that within the IBM world software packages will more and more comply with this CUA guideline. In this case the target was also to join internationally accepted guidelines.

Quality criteria for after-sales service

A well-made mathematical model that has been programmed according to the rules and is sufficiently user-friendly, is not necessarily successful. One of the things that should be well taken care of is the contact between the producer and the user. To be able to maintain contact with the user, provide explanation, answer questions and distribute updates, the producer needs to have an organization to back up the package and to carry out the so-called after-sales activities. This organization takes care of all after-sales service. The after-sales service must guarantee a good relationship between the producer and the consumer. This relationship is important because with the package and the service users must be able to achieve the goals of the company they work for. It therefore affects the effectivity and the efficiency of an organization. Good contact between the producer and the user not only attributes to the success of the package, but will also improve the package quality-wise. The quality criteria which have been formulated for the after-sales service are a first step to the very extensive requirements of the NEN-ISO standards in this field (NEN-ISO, 1988/1989).

It is advisable for both producer and user to put the after-sales activities down in writing by means of a contract. It is a fact that many contracts are more advantageous for the supplier than for the user. Taking this into account, quality criteria for the after-sales service have been drawn up making use of the work of the Home Office of The Netherlands with regard to the drawing up of contracts (Berkvens *et al.*, 1987). Matters that need to be put down in a contract are the documentation and training, the conditions of supply, the linkages, the guarantee and the maintenance.

Quality criteria for after-sales service
Documentation and training
Prices, rates and payments
Conditions of supply
Identification
Duration, termination and current obligations
Guarantee period
Transfer of rights and obligations
Linkages with other packages and hardware
Delivery and installation
Dealing with mutations and problems
Maintenance
Maintenance registration
Configuration management
Change management
Updates

One of the conditions for the successful introduction of software packages is good training of the staff. Not only the operation is important, but also the understanding of the functional working of the package. It must be clear how much training will be given and what the quality of that training will be.

Documentation is expensive, so there must be an agreement whether user manuals will be provided and, if so, how many, and whether the subjects are treated in depth. On bills there is sometimes mention of the fact whether the delivery and payment take place on the basis of the supplier's general conditions of supply. These conditions are usually rather more advantageous for the supplier than for the customer. That is why this article in an agreement should always be overruled by the phrase "Conditions of supply or other conditions of a supplier are not valid in this agreement". Linkages between the various pieces of equipment and other packages prove to cause many problems in practice. It is prudent to include in the agreement that the supplier must solve such problems without extra charges. In the case of software systems supplied from elsewhere, the guarantee period of the supplied system is limited. In this period problems are solved and mistakes are corrected which are detected during this period. They fall under the guarantee clauses of the contract.

Besides the things which have to be laid down in a contract, it is important in what way the communication between the users is realized. One could found a users' club with magazine in which tips and tricks of the package are explained, experiences are discussed and "do's and do not's" are given. The producer too can try to keep in touch with the users through surveys in order to discover their most important requirements.

FUTURE DEVELOPMENTS

The formulated quality criteria and meeting these criteria are the first steps towards standardizing the quality of the mathematical models in the field of air pollution and the software packages which have been developed for this purpose. On the basis of the report "Quality criteria for models to calculate air pollution" (Dekker *et al.*, 1990) the working group on Air Pollution Models under the auspices of the Dutch Standardization Institute (NNI) has drafted a standard on the quality of mathematical models (NNI, 1991). The subjects of quality of software and after-sales have been left aside. In the draft standard for air pollution models qualitative requirements have been layed down for modellers to describe the quality of the model. Per mathematical model these performance characteristics should be filled in quantitatively by the producers of the mathematical models. The publication of the draft standard is planned for September 1991. Such a standard can be called unique because no such standard exists in any field. Already the mentioned report (Dekker *et al.*, 1990) and the draft standard have led to an increased interest and effort to achieve quality by developers of models in The Netherlands.

Via the Dutch Standardization Institute any possible standardization is sure to be inserted in international frameworks like the Comité Européen de Normalisation (CEN) and the International Organisation for Standardization (ISO). This is important because the problem of no quality criteria in the field of (air pollution) mathematical models is international. Unofficially, several representatives from ministries for the environment from other countries, among which are the American and German ministries, have already shown interest in the work that is now being done in this field in The Netherlands.

In this article quality criteria for the GMP of air pollution models have been proposed. Standardization has been set in motion. For the GLP of working with these models, there are no guidelines up to now. The need for these is obvious so they will be formulated sooner or later.

The process of standardization of mathematical models for air pollution has just begun. It is certain, however, that the impulse that has now been given will improve the quality of models which calculate air pollution.

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