Environment Agency Intercomparison Study -Reply to CERC's Comments and Related Matters.

R&D Technical Report P4-078/TR

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Research Contractor: Envirobods Ltd

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Publishing Organisation

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Tel: 01454 624400 Fax: 01454 624409 Website: www.environment-agency.gov.uk

© Environment Agency 2003 March 2003

ISBN 1844321258

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Statement of Use

This report responds to comments by CERC on the intercomparison of regulatory dispersion models described in Environment Agency R&D reports P353 and P362. It also considers more general needs for modelling and models from a regulatory point of view. The information in this document is for use by EA staff and others involved in the regulation of industrial emissions.

Keywords

Dispersion models, intercomparison, AERMOD, ADMS, ISC, Agency regulatory procedures.

Research Contractor

This document was produced under R&D Project P4-078 by: Envirobods Ltd., 13 Badminton Close, Stevenage, Hertfordshire, SG2 8SR.

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EXECUTIVE SUMMARY

This note covers matters related to the intercomparison study of the ADMS, AERMOD and ISC models carried out on behalf of the Environment Agency. It responds to the comments of the work made by CERC at the time.

It also considers the more general aspects of the Agency's needs for modelling and models from a regulatory point of view. Considering the regulatory consequences of dispersion modelling studies, it is, on the whole, surprising how little detailed attention they receive.

There is a need for regulatory models to show minimum standards of compliance of documentation, verification and validation, intercomparison with other models, independent assessment and adequate version control. These might be described as 'verified' models. Other models, which have not achieved this standard but whose use may be needed, might be described as 'unverified' models. It is this compliance that defines the division of models between research activities and regulatory models. The Agency needs to set up a procedural system to achieve this, which should include an element of assessment independent of model developers and suppliers as well as of the Agency. It is, however, important that this process should not inhibit further research and model development.

Previous work in the field of dispersion models for risk assessment, where large numbers of different models have been available, provides a valuable background in the methodologies which are needed for dealing with multiple model use in the public domain. There have also been useful EU initiatives in this area.

There is a larger dimension in this process, which can be applied to numerical models used by the Agency for other purposes. It is also applicable to other dispersion modelling activities in the public domain. A particular case in point at present is the use of models in local authority 'Review and Assessment' procedures for the control of local air quality.

EXECUTIVE SUMMARY

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1. INTRODUCTION

Following the Environment Agency's publication of our dispersion model intercomparison study (Hall et al 2000a, b), CERC Ltd placed a 14-page commentary on the work on their web site (Carruthers et al(2000)) related to their ADMS model and our study's consideration of it. This note is partly a response to that commentary on behalf of the Environment Agency, though the opinions expressed are those of the authors. It also considers other matters related to the study and to the development of model intercomparison and validation procedures in the public domain.

2. BACKGROUND

It seems first to be necessary to explain again the purpose of the original study. This was aimed specifically at the regulatory needs experienced by the Environment Agency in dealing with authorisations using different dispersion models, in particular with the ADMS and AERMOD models and their relationship with the Pasquill/Gifford models, mainly the R91 and ISC models, that preceded them. It was not principally intended to be a detailed critique of the contents of the models or their different approaches to interpreting the physics of the dispersion process, though this inevitably relates to some aspects of the intercomparison study and impinges on their application in regulatory matters.

Regulation with multiple models raises some immediate questions:-

1) Given that regulatory dispersion studies may use any of these models, are there likely to be significant differences between them (from a regulatory point of view) in predicting concentrations to be compared with the required air quality standards for the same application?

2) Is it possible to identify how these differences arise and to account for them in regulatory practice in some simple way?

3) Is there a simple test procedure (or protocol) which would reveal such differences between models? This will also have to satisfy a continuing need to deal with new models and versions of models as they appear, partly so that a historical perspective of the effects of dispersion model changes on regulatory practice can be seen.

The study dealt mainly with these three questions and a number of practical matters associated with them.

The answer to the first question was unhesitatingly yes.

The answer to the second question was that it was only partially possible to do this. Many of the differences between model calculations did not follow consistent patterns and because of the relative internal complexity of the advanced models it was often difficult to see how specific differences between model calculations arose. In answer to the third question we devised a suitable test protocol. It has to be appreciated that its purpose was to reveal any significant differences between regulatory model calculations, not every nuance of their properties. Thus if two models compared using the protocol did not show major differences, it would be unlikely that using them for the same regulatory calculation would show any serious differences. We remain of the view that this should be done with the practicable minimum of calculations, both in the interests of economy and in being able to review relatively quickly any differences between the models being compared. It is very easy in this type of work to become lost in a mass of calculations which are not overall very revealing, since it is often only a few critical results that are important to intercomparisons. Overall, we believe that the test protocol achieved its aims and it has been used subsequently by the Environment Agency's Air Quality Modelling and Assessment Unit for further model intercomparisons (AQMAU(2002)).

3. COMMENTS ON CERC'S RESPONSE

The remarks in this section are headed by the same section numbers as CERC's Note (Carruthers et al(2000)) and are meant to be read in relation to it.

1.3. At the time of writing (and certainly at the date of the reports), the 'older' models (R91 and ISC) remain in heavy use for various purposes, though less so for the Agency's regulatory work. ISC currently remains the standard regulatory model in the USA and worldwide. It was also felt to be important to include them in the study to provide an historical perspective.

1.4. There is less consistency between the newer models than between the older Pasquill/Gifford types, though application of these does differ. The basic equations for the R91 and ISC models are nearly identical. The basic equations for ADMS and AERMOD are not, though they use similar approaches to treating the boundary layer and the basic dispersion parameters within it. They also treat the input meteorological data differently. They are very different in their respective approaches to modelling dispersion over terrain. R91 does not of course attempt to deal with this, though ISC does.

The discussion of the difficulty in estimating boundary layer stability criteria is accepted, but this is an endemic problem with all dispersion calculations with any model. It depends on the point at which you choose to separate the meteorological input from the dispersion calculation. It also applies just as much to determining the Monin-Obukhov length scales and boundary layer heights needed for ADMS and AERMOD which were noted in the intercomparison. This is considered in later comments.

1.5. The reasons for devising an intercomparison protocol with a limited number of test cases are discussed in Section 2. It is also important that a basic protocol be adhered to over time if a historical perspective is to be retained. This does not preclude more detailed comparative studies, but the larger the test data set, the less is the likelihood of its continuing to be used over time and the more difficult it becomes to interpret. There may well be a good case for more detailed data protocols for examining specific aspects of dispersion modelling, building entrainment or plume penetration of the boundary

layer for example. However, in reality this is probably tending more towards research investigations than satisfying a regulatory need. The difference is discussed in Section 4.

1.6. There is a fundamental difference between model intercomparison and other assessments of model performance, including verification and validation studies. The latter are a critical part of model development. Intercomparison is more important in regulatory practice, though clearly it is of general scientific interest whether models purporting to calculate dispersion in similar circumstances produce similar results. The present study was specifically restricted to an intercomparison.

1.7. This touches on a critical matter of potential conflicts of interest between the parties involved in the development of models and the authorisation process using them. It is for model developers and suppliers to ensure as well as they can that their models are physically realistic and their expertise in achieving this is clearly critical. However, independent parties have an essential role to play in providing impartial assessments of models. This is widely recognised in other modelling areas, such as hazard assessment, where a multiplicity of models has reigned for many years and the need for impartial assessment has been more obvious. It is discussed in more detail by Britter(1991) and others and the point is considered in more detail in the Discussion to this note (Section 4). The need for such independent assessments is also noted in the Royal Meteorological Society's guidance (Roy. Met Soc (1995)).

2.1. Whatever discussion there has been during the development and use of ADMS, this list is essentially of 'closed' meetings and not of publicly accessible information, which in the long run is what has to be provided for a model used in the public domain.

2.2. The review of previous model intercomparisons included all that could be found, partly as there were so few of these. The improvements over time of different versions of ADMS used in the studies may well be real, but so poor was the background information delivered with new model versions during the period that the nature and effect of changes in the model were difficult, if not impossible to discern. The discussion in the review document makes this point. Any improvements to the model due to discussions over Jones et al's(1995) work were not mentioned as they were never made public. It is difficult under these circumstances to refer to them.

2.3. The intercomparison study was effectively completed before the revised technical specification documents appeared on the CERC web site. The study and its comments were based on what was available at the time and the remarks on this stand. The revised CERC documentation does represent a considerable improvement on the earlier versions.

2.4. The question is not one of the improvement or development of models, including ADMS, but of the effective documentation of the nature and effects of these changes. We regard this as particularly critical for regulatory models on which substantial consequences may hinge. Irrespective of what may be the merits of ADMS, this aspect of its development has been seriously lacking in the past.

2.5/2.6. The API study (Hanna et al(1999)) was not perfectly independent as many of the dispersion calculations were devolved to the model developers.

With regard to the quality of the intercomparison statistics, it has to be borne in mind that due to the high levels of scatter in the intercomparison field data sets, this sort of assessment simply cannot be made with great accuracy. The outcome of the work as expressed in Tables 6 and 7 from Hanna et al's work was that overall there did seem to be significant differences between the quality of agreement with the data between the ISC model on one hand and the ADMS and AERMOD models on the other. Differences between the statistics of the fit of the ADMS and AERMOD models to the data were relatively much smaller. Though the numerical balance of comparison values lay with ADMS, the differences between the parameter values for ADMS and AERMOD are probably within the order of accuracy with which this sort of comparison can be made.

2.6/3.1. Though the API may have recommended that ADMS be adopted as a regulatory model in the USA, the general opinion seems to be that the prospect of its doing so remains remote unless its content is made much more transparent and its basic model effectively becomes open source.

The status of AERMOD is that it is generally accepted to be EPA's putative improved standard dispersion model (irrespective of its formal classification) and it is at present progressing steadily through the long process of being accepted as such in the US. At the time of writing it seems most likely that it will be formally accepted as the EPA's standard industrial source dispersion model around the middle of 2003.

The incorporation of the PRIME building downwash model into AERMOD is also under consideration, though at present more slowly. At the time it was not available for use in the intercomparison study. PRIME is now available for use with AERMOD from some model suppliers, but (unusually for the USA) is currently not properly documented and no significant description of its content or performance has been issued. This omission will clearly have to be rectified before it can be more generally accepted.

4.1-4.3. Meteorology. An assessment of the meteorological pre-processors was not a formal part of the intercomparison study, these being largely regarded as integral parts of the different models. However, their critical importance became apparent during the study and their behaviour was briefly investigated. This was sufficient to show the need for a much more careful assessment of the process of converting raw meteorological data to the essential input parameters for dispersion calculations and that the ADMS and AERMOD pre-processors could produce quite different estimates of the state of the boundary layer.

The need for further investigation and research in this area seems self evident, especially (as noted in the study) since differences in the meteorological data processing may be at least as critical to differences between model calculations as the dispersion calculations themselves. There are more general related problems of model reliability in this area, such as the effects of disequilibrium in the boundary layer (its most common state) and the accuracy and reliability of meteorological data generally and its effects on dispersion calculations.

5. Briggs' formulations for plume rise are by far the most commonly used for point sources, probably with good reason as all the evidence is that, though relatively simple,

they work fairly well. In using its alternative recursive calculation the ADMS model is relatively unusual for industrial discharge calculations. More complex plume rise models are used for more complex problems, as in HG-System, which is intended to deal with far more complex and varied releases including heavier-than-air gases. A difficulty with these more complex plume rise procedures is in verifying them, as additional parameters are used beyond the Briggs formulations.

The problems and uncertainties in estimating plume penetration of the boundary layer are very real, but can be of critical importance in calculations for large buoyant releases such as power stations. However, their reliability is little discussed and the fraction of the plume penetrating the boundary layer is an important parameter in these cases.

6. Building Effects.

The critical feature of dispersion around buildings in the near field (that is within about 10-20 building heights or widths, whichever is the smaller) is its great sensitivity to the details of the structure and the orientation of the approach flow. No relatively simple model (as were, in varying degrees, all the models in the intercomparison study) can predict this behaviour reliably. This is especially so if, as is the case here, many of the phenomena associated with building aerodynamics and the subsequent plume entrainment are ignored. At best it is possible to give a general indication of the concentrations that might prevail in this region. In this sense all the building models investigated in the intercomparison study, as well as PRIME, must be classed as relatively primitive representations of reality as compared with, say, the gaussian plume in open terrain (itself an approximation to reality). The initial treatment of buildings in the models, converting them (whether singly or in groups) to the nearest equivalent rectangular block irrespective of what effect this may have on the dispersion patterns, is indicative of the level of modelling used.

At longer distances, away from the near field, the local details of the building aerodynamics become less important and there is a greater possibility of more reliable prediction. AERMOD and ISC only operate in this region, whereas ADMS and PRIME carry out a limited near-field calculation. ADMS partitions the plume into entrained and unentrained fractions, the former of which provides an estimate of the concentration in the separated wake. Since this is still based on the approximation of the building (or buildings) into the nearest plain rectangular block, this cannot in general be very precise. The plume partitioning (itself difficult to do accurately) represents a process that occurs in practice, but is in reality more diffuse than the dichotomy that the ADMS model assumes. As a result, it tends in the near-field to generate a much sharper effect due to the two-part plume than actually occurs. It is only when the two plumes have merged more at longer distances (typically those beyond 10-20 building heights) that the prediction becomes more reliable.

Though it was not included in the original study (the model was not yet available) this sort of criticism almost certainly extends to PRIME. However, the methodology of PRIME has yet to be clearly described, so it is difficult to consider it in any detail.

The development of the ADMS building module to incorporate effects noted in Sections 6.4 and 6.5 are to be welcomed. That related to Harvey's experiments in Section 6.4 occurred after the publication of the intercomparison. A more general criticism must

be that, as with many modifications to the ADMS model, these changes have only been discussed within small groups or by direct contact and have rarely been circulated more widely. It is important for all users to know both what changes have been made to a model and what effects they may have on any calculation.

7. Complex terrain.

We made it quite clear in the original reports that there were fundamental differences between ADMS and AERMOD/ISC in modelling over terrain. One (ADMS) calculates a modified wind field related to the terrain, followed by a dispersion calculation. The others (AERMOD/ISC) use an empirical correction (based on the terrain) to the calculated concentration in flat terrain. Our main concern was the differences in calculated concentrations resulting from these approaches. We did not investigate dispersion behaviour on the lee side of the hill as this is only critically important with very stable flows, where this flow behaviour is complex. It was felt to be still in the stage of research studies and seemed likely to be beyond the abilities of any current regulatory dispersion model. It is an example of cases that might be considered in more detailed assessments of specific aspects of model behaviour, rather than the basic overall test protocol used in the study.

The question of terrain and calculation grids is really a matter for the individual model's internal procedures. The user is interested in the calculated concentrations at his chosen output grid, which was selected to be the same for each of the models. As far as possible terrain information was also supplied at a fixed resolution to the different models. That used for ADMS in the intercomparison was at 64 x 64 resolution for the single case runs (4096 points, the maximum possible) and 32x32 for the annual runs (the recommended values, in order to avoid extremely long run times). It seems unhelpful to suggest that, because the data input arrangements and calculation procedures of ADMS and AERMOD are different, comparison of their respective outputs is impracticable.

4. DISCUSSION

The models investigated in the intercomparison study are used in critical aspects of regulatory assessments of many process and combustion plant emissions. They are used to assess potential human health effects and ecological damage due to ambient pollutants and to predict the possibilities of exceeding prescribed air quality standards. The industrial, economic and social consequences of decisions based on these assessments can be considerable, including, for example, whether a major process plant or generating unit may be authorised at all, or with a requirement for abatement equipment whose cost may be of the order of £100M.

Under these circumstances it might be expected that, in the interests of consistent regulation, close attention would be given to the accuracy and reliability of such models and additionally to their relative performance. Since this is also a matter in the public domain for which there is a wide public interest, such matters should be as transparent and disinterested as possible. It also seems clear that when the results of model calculations exert such an influence, they are too important a matter to be left to the model developers and suppliers, or the regulators, alone.

The formal process of validation and verification of models requires the model developer to ensure as well as he can that his model satisfies its described physics and that the numerical code executes this. There is also a requirement for full documentation of the model's methodology. Following this there should be a requirement for disinterested assessment of the model's physics and its numerical code, including sample calculations against standard test protocols. Where there are several models of a particular type a common intercomparison process is also needed. This is regarded as standard practice in most fields of application of numerical models of physical processes. It is discussed, amongst other places, in the Royal Meteorological Society's guidance (Roy. Met. Soc. (1995)). The EC Model Evaluation Group(1994a,b, 1995) has also issued guidelines on model evaluation and development.

In some areas of dispersion modelling, especially in hazard assessment where there has been a multiplicity of models, consideration of model evaluation and assessment has received detailed attention from an early date. Britter(1991) discussed the evaluation of hazardous accident models and considered both the philosophy and the methodologies of the process. Others have produced methodologies and carried out detailed intercomparison studies. Hanna et al(1991), for example, devised a methodology and tested fourteen current heavy gas models, one of the first such examples of thorough multiple dispersion model assessment. More recently the EU SMEDIS project (SMEDIS(2000), Carrissimo et al(2000), Daish et al (2000)) has laid down a detailed methodology and procedural protocol for heavy gas dispersion model assessment. Both Britter and Hanna et al comment on the importance of independent disinterested model assessment and peer review as part of the evaluation process.

The AERMOD, ISC and ADMS models have been subject to published verification procedures by their developers (the bibliography in the intercomparison study review lists many of these papers) and there has been a significant effort in providing standardised test data (for example the Model Validation Kit (Olesen(1996, 1999)), much of which can be found in the Proceedings of the various HARMO conferences. Some of the methodology developed for this has used techniques derived from the earlier work on risk assessment models, for example the statistical parameters used by Hanna et al(1991).

For industrial source models in the UK, the later stages of this process of independent assessment and intercomparison have been a rather limited activity and there has been a tendency to accept models as 'given'. Apart from Carruthers et al's(1996) work on comparing different model calculations with LIDAR data, the present intercomparison has been the first major (and the sole independent) openly published multi-model comparison in this regulatory area. Considering the commonplace use of these procedures in other regulatory areas, this seems surprising, as does the reaction it has generated. Some historical continuity in model intercomparison is now developing, as part of the present protocol has now been used again to examine recent revisions in ADMS and AERMOD (AQMAU(2002)).

It would clearly be desirable for there to be a better established procedure for assessing and accepting industrial source dispersion models for regulatory use in the UK. The protocol devised for the intercomparison study provides a useful test methodology for this, but should be part of a wider ranging assessment methodology. The procedures in use and under consideration for risk assessment models, noted above, provide a good basis for this. In the first instance it would be useful for the regulatory authorities to place on regulatory models minimum standards of compliance with acceptable good practice if they are to be used. These might include:

- Adequate documentation and a full description of the physical processes modelled.
- Evidence of adequate verification and validation studies, comparing the model calculations with known standard and other experimental test data.
- Intercomparison with other models against standard test protocols, so that any differences in performance can be clearly seen.
- Adequate independent peer review and assessment.
- Effective 'version control'. That is, the provision of adequate documentation on revised versions of the same model, together with intercomparison calculations (using at least the standard test protocol) clearly indicating the effects of any changes on model calculations.

All this information should be openly available to any interested parties, preferably via the Web. Publication of related studies in the peer-reviewed literature would be preferred.

It is surprising that in many ways relatively little attention is given to such regulatory needs, especially considering that the main (indeed almost the sole) purpose of these models is regulatory practice. Not all currently available models satisfy even these basic requirements. At the time of writing, for example, the PRIME building downwash model, included as an adjunct to AERMOD by some suppliers of this model, fails most of these requirements and is at present very poorly documented.

Hanna et al recommended the setting up of peer review groups as part of the process of independent assessment of models. This may well have its place in the process, though it is not without its own dangers as members of peer review committees can be subject to conflicts of interests. The question of what constitutes 'independent assessment' is also somewhat open, including the role of the Agency itself. As an 'interested party' in the regulatory process, it may lay itself open to accusations of self interest if it takes upon itself the process of model assessment. In the intercomparison report it was recommended that the continuing process of intercomparison and model assessment should be independent of both the model developers and suppliers and of the Agency itself. We remain of this view and feel that the Agency would serve itself better by adopting a slightly detached view of the process.

This discussion has mainly centred on the questions of model verification and control for regulatory use, since this is presently the greatest deficiency in regulatory dispersion modelling. However, it remains desirable to balance the respective needs of scientific model development and regulatory practice. Despite the effort that has gone into their development, all practical dispersion models remain limited approximations to the physical processes involved. There is unquestionably considerable scope for their further scientific development and improvement and in the long run it would be detrimental if this process were inhibited. The intercomparison of different models against a common protocol is only the first part of the scientific process which ought to accompany dispersion model development and use. What should follow from this is more detailed investigation of the causes of the differences between models, whether due to numerical, scientific or other causes, that will result in improvements in modelling techniques.

A main cause of the difficulty that has arisen in this process is in the passage of models from the research activities involved in their development to their application in regulatory practice. Dispersion models are not exact; they are essentially in the class of application of approximate semi-empirical models dealing with calculations associated with relatively high levels of uncertainty. During their scientific development it is quite common for the values of 'constants' to be altered, methods of numerical solution modified or the scientific balance of different components of the calculation to be These may be for scientific or computational reasons, in the interests of revised. 'improving' the model. Any of these changes may also alter the output of the model calculations, but if the changes are within the bounds of the uncertainties and their physical and numerical properties are described, this is, in a scientific sense, quite fair and reasonable. It is less fair and reasonable if such changes are arbitrarily passed through to the regulatory use of the model, in view of the alteration to regulatory judgements and substantial economic and social effects that may result. It is at this bridge between scientific development and regulatory use that minimum standards of compliance of the model with the regulatory need should be applied. It is, presently in the UK, this boundary that is inadequately defined and controlled.

5. RECOMMENDATIONS FOR FURTHER WORK ON REGULATORY MODELLING METHODS.

There is a need for the Agency to lay down minimum scientific, numerical and documentary requirements, based on the list above and other work in this field, for dispersion models that are fully acceptable for use in regulatory practice. This is not a matter of 'prescription' of models, which the Agency does not undertake, but of satisfying minimum acceptable standards for their regulatory use. There is also a need for an Agency organisational structure to deal with these matters. Models that satisfy these requirements might be described as 'verified'. There may also clearly be a need to use models which deal with matters of technical interest, but which have yet to satisfy these requirements. Models of this type might be described as 'unverified' and their results treated with greater caution than with 'verified' models.

The description of a model as 'verified' does not imply that its output is necessarily an accurate estimate of what it purports to model. It does, however, imply that it has been subject to what verification and validation is practicable, what it models is clearly described and understood and that the software reproduces the physical process described in its technical documentation.

There remains a need for an element in this process which is independent of the model developers and suppliers and of the Agency.

There is almost certainly a wider need for the application of this process by the Agency

to numerical models used for regulatory purposes in other fields. An overarching Agency document related to this matter, on which detailed practice in assessing models in different fields could be based, would be desirable.

Beyond the immediate requirements of the Agency in this area, there is a wider UK dimension for this process. One clear example is the use of dispersion models by Local Authorities in the 'Review and Assessment' process for local air pollution control. Here the situation is in many ways similar to that with industrial source models. They are used to assess potential human health effects and ecological damage due to ambient pollutants and to predict the possibilities of exceeding prescribed air quality standards. The industrial, economic and social consequences of decisions based on these assessments can be considerable. They affect planning decisions on site developments and on transport, including the development of roads and restrictions in use of existing roads. The declaration of Air Quality Management Areas, especially, can significantly affect local land use and property values. The process is in the public domain and the results are of wide public interest. Despite this, independent assessment of the models used and their relative performance has been minimal. There are at present three different models in use for this work, none of which has been subject to independent assessment. Nor has there been any intercomparison of their relative performance in the Review and Assessment process.

6. CONCLUSIONS

This note covers matters related to the intercomparison study of the ADMS, AERMOD and ISC models carried out on behalf of the Environment Agency. It has responded to the comments on the work by CERC at the time.

It has also considered the more general aspects of the Agency's needs for modelling and models from a regulatory point of view. Considering the regulatory consequences of dispersion modelling studies, it is, on the whole, surprising how little detailed attention these receive.

There is a need for regulatory models to show minimum standards of compliance of documentation, verification and validation against experimental test data, intercomparison with other models, independent assessment and adequate version control. These might be described as 'verified' models. Other models which have not achieved this standard but whose use may be needed, might be described as 'unverified' models. It is this compliance that should define the boundary of models between research activities and regulatory models. The Agency needs to set up a procedural system to achieve this, which should include an element of assessment independent of model developers and suppliers as well as of the Agency. However, it is important that this process should not inhibit further research and model development.

There is a larger dimension in this process, which can be applied to numerical models used by the Agency for other purposes. It is also applicable to other dispersion modelling activities in the public domain. A particular case in point at present is the use of models in local authority 'Review and Assessment' procedures for the control of local air quality.

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