INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

UNITED NATIONS INDUSTRIAL DEVELOPMENT ORGANIZATION

INTERNATIONAL CENTRE FOR SCIENCE AND HIGH TECHNOLOGY
c/o INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS 34100 TRIESTE (ITALY) VIA GRIGNANO, 9 (ADRIATICO PALACE) P.O. BOX 586 TELEPHONE 040-224572 TELEFAX 040-224575 TELEX 460449 APH I

SMR/760-3

"College on Atmospheric Boundary Layer and Air Pollution Modelling"
16 May - 3 June 1994

SUPPLMENT B
to the
"Guideline on Air Quality Models (Revised)"

presented by:
S. HANNA
Environmental Research and Technology, Inc.
Concord, Massachusetts
USA

Please note: These notes are intended for internal distribution only.

12

DiCristofaro

SUPPLEMENT B

TO THE

GUIDELINE ON AIR QUALITY MODELS (REVISED)

(Appendix W of 40 CFR Part 51)

FEBRUARY 1993

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Radiation
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina 27711

PREFACE

Industry and control agencies have long expressed a need for consistency in the application of air quality models for regulatory purposes. In the 1977 Clean Air Act, Congress mandated such consistency and encouraged the standardization of model applications. The Guideline on Air Quality Models was first published in April 1978 to satisfy these requirements by specifying models and providing guidance for their use. This guideline provides a common basis for estimating the air quality concentrations used in assessing control strategies and developing emission limits.

The continuing development of new air quality models in response to regulatory requirements and the expanded requirements for models to cover even more complex problems have emphasized the need for periodic review and update of guidance on these techniques. Four primary on-going activities provide direct input to revisions of this modeling guideline. The first is a series of annual EPA workshops conducted for the purpose of ensuring consistency and providing clarification in the application of models. The second activity, directed toward the improvement of modeling procedures, is the cooperative agreement that EPA has with the scientific community represented by the American Meteorological Society. This agreement provides scientific assessment of procedures and proposed techniques and sponsors workshops on key technical issues. The third activity is the solicitation and review of new models from the technical and user community. In the March 27, 1980 Federal Register, a procedure was outlined for the submittal to EPA of privately developed models. After extensive evaluation and scientific review, these models, as well as those made available by EPA, are considered for recognition in this guideline. The fourth activity is the extensive on-going research efforts by EPA and others in air quality and meteorological modeling.

Based primarily on these four activities, this document embodies revisions to the "Guideline on Air Quality Models." Although the text has been revised from the 1978 guide, the present content and topics are similar. As necessary, new sections and topics are included. EPA does not make changes to the guidance on a predetermined schedule, but rather on an as needed basis. EPA believes that revisions to this guideline should be timely and responsive to user needs and should involve public participation to the greatest possible extent. All future changes to the guidance will be proposed and finalized in the Federal Register. Information on the current status of modeling guidance can always be obtained from EPA's Regional Offices.

TABLE OF CONTENTS

Page

Page

TABLE 4-1

Preferred Models for Selected Applications in Simple Terrain

Short Term (i.e., 1-24 hours)	Land Use	Model[1]
Single Source	Rural Urban	CRSTER RAM
Multiple Source	Rural Urban	MPTER RAM
Complicated Sources[2]	Rural/Urban	ISCST2
Buoyant Industrial Line Sources	Rural	BLP
Long Term (i.e., monthly, seasonal or annual)		
Single Source	Rural Urban	CRSTER RAM
Multiple Source	Rural Urban	MPTER CDM 2.0 or RAM[3]
Complicated Sources[2]	Rural/Urban	ISCLT2
Buoyant Industrial Line Sources	Rural	BLP

[1]Several of these models contain options which allow them to be interchanged. For Example, ISCST2 can be substituted for CRSTER and equivalent, if not identical, concentration estimates obtained. Similarly, for a point source application, MPTER with urban option can be substituted for RAM. Where a substitution is convenient to the user and equivalent estimates are assured, it may be made. The models as listed here reflect the applications for which they were originally intended.

[2]Complicated sources are those with special problems such as aerodynamic downwash, particle deposition, volume and area sources, etc.

[3]If only a few sources in an urban area are to be modeled, RAM should be used.

5.0 MODEL USE IN COMPLEX TERRAIN

5.1 Discussion

For the purpose of this guideline, complex terrain is defined as terrain exceeding the height of the stack being modeled. Complex terrain dispersion models are normally applied to stationary sources of pollutants such as SO_2 and particulates.

A major outcome from the EPA Complex Terrain Model Development project has been the publication of a refined dispersion model (CTDM) suitable for regulatory application to plume impaction assessments in complex terrain.[21] Although CTDM as originally produced was only applicable to those hours characterized as neutral or stable, a computer code for all stability conditions, CTDMPLUS,[19] together with a user's guide,[22] and on-site meteorological and terrain data processors,[23,24] is now available. Moreover, CTSCREEN,[19,25] a version of CTDMPLUS that does not require on-site meteorological data inputs, is also available as a screening technique.

The methods discussed in this section should be considered in two categories: (1) screening techniques, and (2) the refined dispersion model, CTDMPLUS, discussed below and listed in Appendix A.

Continued improvements in ability to accurately model plume dispersion in complex terrain situations can be expected, e.g., from research on lee side effects due to terrain obstacles. New approaches to improve the ability of models to realistically simulate atmospheric physics, e.g., hybrid models which incorporate an accurate wind field analysis, will ultimately provide more appropriate tools for analyses. Such hybrid modeling techniques are also acceptable for regulatory applications after the appropriate demonstration and evaluation.[15]

6.2 Recommendations

6.2.1 Models for Ozone

The Urban Airshed Model (UAM)[19,28] is recommended for photochemical or reactive pollutant modeling applications involving entire urban areas. To ensure proper execution of this numerical model, users must satisfy the extensive input data requirements for the model as listed in Appendix A and the users guide. Users are also referred to the "Guideline for Regulatory Application of the Urban Airshed Model"[29] for additional data requirements and procedures for operating this model.

The empirical model, City-specific EKMA,[19,30-33] has limited applicability for urban ozone analyses. Model users should consult the appropriate Regional Office on a case-by-case basis concerning acceptability of this modeling technique.

Appendix B contains some additional models that may be applied on a case-by-case basis for photochemical or reactive pollutant modeling. Other photochemical models, including multi-layered trajectory models, that are available may be used if shown to be appropriate. Most photochemical dispersion models require emission data on individual hydrocarbon species and may require three dimensional meteorological information on an hourly basis. Reasonably sophisticated computer facilities are also often required. Because the input data are not universally available and studies to collect such data are very resource intensive, there are only limited evaluations of those models.

For those cases which involve estimating the impact on ozone concentrations due to stationary sources of VOC and NO_x, whether for permitting or other regulatory cases, the model user should consult the appropriate Regional Office on the acceptability of the modeling technique.

Proportional (rollback/forward) modeling is not an acceptable procedure for evaluating ozone control strategies.

6.2.2 Models for Carbon Monoxide

For analyzing CO impacts at roadway intersections, users should follow the procedures in the "Guideline for Modeling Carbon Monoxide from Roadway Intersections".[34] The recommended model for such analyses is CAL3QHC.[35] This model combines CALINE3 (already in Appendix A) with a traffic model to calculate delays and queues that occur at signalized intersections. In areas where the use of either TEXIN2 or CALINE4 has previously been established, its use may continue. The capability exists for these intersection models to be used in either a screening or refined mode. The screening approach is described in reference 34; a refined approach may be considered on a case-by-case basis. The latest version of the MOBILE (mobile source emission factor) model should be used for emissions input to intersection models.

For analyses of highways characterized by uninterrupted traffic flows, CALINE3 is recommended, with emissions input from the latest version of the MOBILE model.

The recommended model for urban areawide CO analyses is RAM or Urban Airshed Model (UAM); see Appendix A. Information on SIP development and requirements for using these models can be found in references 34, 96, 97 and 98.

Where point sources of CO are of concern, they should be treated using the screening and refined techniques described in Section 4 or 5 of the Guideline.

7.2.2 Particulate Matter

The new particulate matter NAAQS, promulgated on July 1, 1987 (52 FR 24634), includes only particles with an aerodynamic diameter less than or equal to a nominal 10 micrometers (PM-10). EPA has also proposed regulations for PSD increments measured as PM-10 in a notice published on October 5, 1989 (54 FR 41218).

Screening techniques like those identified in Section 4 are also applicable to PM-10 and to large particles. It is recommended that subjectively determined values for "half-life" or pollutant decay not be used as a surrogate for particle removal. Conservative assumptions which do not allow removal or transformation are suggested for screening. Proportional models (rollback/forward) may not be applied for screening analysis, unless such techniques are used in conjunction with receptor modeling.

Refined models such as those in Section 4 are recommended for PM-10 and large particles. However, where possible, particle size, gas-to-particle formation, and their effect on ambient concentrations may be considered. For urban-wide refined analyses CDM 2.0 or RAM should be used. CRSTER and MPTER are recommended for point sources of small particles. For source-specific analyses of complicated sources, the ISC2 model is preferred. No model recommended for general use at this time accounts for secondary particulate formation or other transformations in a manner suitable for SIP control strategy demonstrations. Where possible, the use of receptor models[38,39,105,106,107] in conjunction with dispersion models is encouraged to more precisely characterize the emissions inventory and to validate source specific impacts calculated by the dispersion model. A SIP development guideline,[108] model reconciliation guidance,[106] and an example model application[109] are available to assist in PM-10 analyses and control strategy development.

Under certain conditions, recommended dispersion models are not available or applicable. In such circumstances, the modeling approach should be approved by the appropriate Regional Office on a case-by-case basis. For example, where there is no recommended air quality model and area sources are a predominant component of PM-10, an attainment demonstration may be based on rollback of the apportionment derived from two

7.2.4 Visibility

The visibility regulations as promulgated in December 1980 require consideration of the effect of new sources on the visibility values of Federal Class I areas. The state of scientific knowledge concerning identifying, monitoring, modeling, and controlling visibility impairment is contained in an EPA report "Protecting Visibility: An EPA Report to Congress".[42] In 1985, EPA promulgated Federal Implementation Plans (FIPs) for states without approved visibility provisions in their SIPs. A monitoring plan was established as part of the FIPs.[b]

Guidance and a screening model, VISCREEN, is contained in the EPA document "Workbook for Plume Visual Impact Screening and Analysis (Revised)."[43] VISCREEN can be used to calculate the potential impact of a plume of specified emissions for specific transport and dispersion conditions. If a more comprehensive analysis is required, any refined model should be selected in consultation with the EPA Regional Office and the appropriate Federal Land Manager who is responsible for determining whether there is an adverse effect by a plume on a Class I area.

PLUVUE II, listed in Appendix B, may be applied on a case-by-case basis when refined plume visibility evaluations are needed. Plume visibility models have been evaluated against several data sets.[44,45]

---

[b] 40 CFR 51.300-307

A.5 INDUSTRIAL SOURCE COMPLEX MODEL (ISC2)

Reference: Environmental Protection Agency, 1992. User's Guide for the Industrial Source Complex (ISC2) Dispersion Models, Volumes 1, 2, and 3. EPA Publication Nos. EPA-450/4-92-008a-c. Environmental Protection Agency, Research Triangle Park, NC. (NTIS Nos. PB 92-232461, PB 92-232453, and PB 92-232479, respectively)

Availability: The model code is available on the Support Center for Regulatory Air Models Bulletin Board System and also from the National Technical Information Service (see page A-1).

Abstract: The ISC2 model is a steady-state Gaussian plume model which can be used to assess pollutant concentrations from a wide variety of sources associated with an industrial source complex. This model can account for the following: settling and dry deposition of particles; downwash; area, line and volume sources; plume rise as a function of downwind distance; separation of point sources; and limited terrain adjustment. It operates in both long-term and short-term modes.

a. Recommendations for Regulatory Use

ISC2 is appropriate for the following applications:

- industrial source complexes;
- rural or urban areas;
- flat or rolling terrain;
- transport distances less than 50 kilometers;
- 1-hour to annual averaging times; and

- continuous toxic air emissions.

The following options should be selected for regulatory applications:

For short term or long term modeling, set the regulatory "default option"; i.e., use the keyword DFAULT, which automatically selects stack tip downwash, final plume rise, buoyancy induced dispersion (BID), the vertical potential temperature gradient, a treatment for calms, the appropriate wind profile exponents, the appropriate value for pollutant half-life, and a revised building wake effects algorithm; set the "rural option" (use the keyword RURAL) or "urban option" (use the keyword URBAN); and set the "concentration option" (use the keyword CONC).

b. Input Requirements

Source data: location, emission rate, physical stack height, stack gas exit velocity, stack inside diameter, and stack gas temperature. Optional inputs include source elevation, building dimensions, particle size distribution with corresponding settling velocities, and surface reflection coefficients.

Meteorological data: ISCST2 requires hourly surface weather data from the preprocessor program RAMMET, which provides hourly stability class,wind direction, wind speed, temperature, and mixing height. For ISCLT2, input includes stability wind rose (STAR deck), average afternoon mixing height, average morning mixing height, and average air temperature.

Receptor data: coordinates and optional ground elevation for each receptor.

c. Output

Printed output options include:

- program control parameters, source data, and receptor data;
- tables of hourly meteorological data for each specified day;
- "N"-day average concentration or total deposition calculated at each receptor for any desired source combinations;
- concentration or deposition values calculated for any desired source combinations at all receptors for any specified day or time period within the day;
- tables of highest and second highest concentration or deposition values calculated at each receptor for each specified time period during a(n) "N"-day period for any desired source combinations, and tables of the maximum 50 concentration or deposition values calculated for any desired source combinations for each specified time period.

d. Type of Model

ISC2 is a Gaussian plume model.

e. Pollutant Types

ISC2 may be used to model primary pollutants and continuous releases of toxic and hazardous waste pollutants. Settling and deposition are treated.

f. Source-Receptor Relationships

ISC2 applies user-specified locations for point, line, area and volume sources, and user-specified receptor locations or receptor rings.

User input topographic evaluation for each receptor is used. Elevations above stack top are reduced to the stack top elevation, i.e., "terrain chopping".

User input height above ground level may be used when necessary to simulate impact at elevated or "flag pole" receptors, e.g., on buildings.

Actual separation between each source-receptor pair is used.

g. Plume Behavior

ISC2 uses Briggs (1969, 1971, 1975) plume rise equations for final rise.

Stack tip downwash equation from Briggs (1974) is used.

Revised building wake effects algorithm is used. For stacks higher than building height plus one-half the lesser of the building height or building width, the building wake algorithm of Huber and Snyder (1976) is used. For lower stacks, the building wake algorithm of Schulman and Scire (Schulman and Hanna, 1986) is used, but stack tip downwash and BID are not used.

For rolling terrain (terrain not above stack height), plume centerline is horizontal at height of final rise above source.

Fumigation is not treated.

h. Horizontal Winds

Constant, uniform (steady-state) wind is assumed for each hour.

Straight line plume transport is assumed to all downwind distances.

Separate wind speed profile exponents (EPA, 1980) for both rural and urban cases are used.

An optional treatment for calm winds is included for short term modeling.

i. Vertical Wind Speed

Vertical wind speed is assumed equal to zero.

A.8 URBAN AIRSHED MODEL (UAM)

References: Environmental Protection Agency, 1990. User's Guide for the Urban Airshed Model, Volume I-VIII. EPA Publication Nos. EPA-450/4-90-007a-c, d(R), e-g, and EPA-454/B-93-004, respectively. U.S. Environmental Protection Agency, Research Triangle Park, NC (NTIS Nos. PB 91-131227, PB 91-131235, PB 91-131243, PB 93-122380, PB 91-131268, PB 92-145382, and PB 92-224849, respectively, for Vols. I-VII).

Availability: The model code is available on the Support Center for Regulatory Air Models Bulletin Board System and also from the National Technical Information Service (see page A-1).

Abstract: UAM is an urban scale, three dimensional, grid type numerical simulation model. The model incorporates a condensed photochemical kinetics mechanism for urban atmospheres. The UAM is designed for computing ozone (O_3) concentrations under short-term, episodic conditions lasting one or two days resulting from emissions of oxides of nitrogen (NO_x), volatile organic compounds (VOC), and carbon monoxide (CO). The model treats urban VOC emissions as their carbon-bond surrogates.

a. Recommendations for Regulatory Use

UAM is appropriate for the following applications: urban areas having significant ozone attainment problems and one hour averaging times.

UAM has many options but no specific recommendations can be made at this time on all options. The reviewing agency

should be consulted on selection of options to be used in regulatory applications.

b. Input Requirements

Source data: gridded, hourly emissions of PAR, OLE, ETH, XYL, TOL, ALD2, FORM, ISOR, ETOTH, MEOH, CO, NO, and NO_2 for low-level sources. For major elevated point sources, hourly emissions, stack height, stack diameter, exit velocity, and exit temperature.

Meteorological data: hourly, gridded, divergence free, u and v wind components for each vertical level; hourly gridded mixing heights and surface temperatures; hourly exposure class; hourly vertical potential temperature gradient above and below the mixing height; hourly surface atmospheric pressure; hourly water mixing ratio; and gridded surface roughness lengths.

Air quality data: concentration of all carbon bond 4 species at the beginning of the simulation for each grid cell; and hourly concentrations of each pollutant at each level along the inflow boundaries and top boundary of the modeling region.

Other data requirements are: hourly mixed layer average, NO_2 photolysis rates; and ozone surface uptake resistance along with associated gridded vegetation (scaling) factors.

c. Output

Printed output includes:

- gridded instantaneous concentration fields at user-specified time intervals for user-specified pollutants and grid levels;
- gridded time-average concentration fields for user-specified time intervals, pollutants, and grid levels.

d. Type of Model

UAM is a three dimensional, numerical, photochemical grid model.

e. Pollutant Types

UAM may be used to model ozone (O_3) formation from oxides of nitrogen (NO_x) and volatile organic compound (VOC) emissions.

f. Source-Receptor Relationship

Low-level area and point source emissions are specified within each surface grid cell. Emissions from major point sources are placed within cells aloft in accordance with calculated effective plume heights.

Hourly average concentrations of each pollutant are calculated for all grid cells at each vertical level.

g. Plume Behavior

Plume rise is calculated for major point sources using relationships recommended by Briggs (1971).

h. Horizontal Winds

See Input Requirements.

i. Vertical Wind Speed

Calculated at each vertical grid cell interface from the mass continuity relationship using the input gridded horizontal wind field.

j. Horizontal Dispersion

Horizontal eddy diffusivity is set to a user specified constant value (nominally 50 m^2/s).

k. Vertical Dispersion

Vertical eddy diffusivities for unstable and neutral conditions calculated using relationships of Lamb et al. (1977); for stable conditions, the relationship of Businger and Arya (1974) is employed. Stability class, friction velocity, and Monin-Obukhov length determined using procedure of Liu et al. (1976).

l. Chemical Transformation

UAM employs a simplified version of the Carbon-Bond IV Mechanism (CBM-IV) developed by Gery et al. (1988) employing various steady state approximations.

m. Physical Removal

Dry deposition of ozone and other pollutant species are calculated. Vegetation (scaling) factors are applied to the reference surface uptake resistance of each species depending on land use type.

n. Evaluation Studies

Builtjes, P. J. H., K. D. van der Hurt, and S. D. Reynolds, 1982. Evaluation of the Performance of a Photochemical Dispersion Model in Practical Applications, 13th International Technical Meeting on Air Pollution Modeling and Its Application, Ile des Embiez, France.

Cole, H. S., D. E. Layland, G. K. Moss, and C. F. Newberry, 1983. The St. Louis Ozone Modeling Project. EPA Publication No. EPA-450/4-83-019. U.S. Environmental Protection Agency, Research Triangle Park, NC.

Dennis, R. L., M. W. Downton, and R. S. Keil, 1983. Evaluation of

B.0 INTRODUCTION AND AVAILABILITY

This appendix summarizes key features of refined air quality models that may be considered on a case-by-case basis for individual regulatory applications. For each model, information is provided on availability, approximate cost in 1990, regulatory use, data input, output format and options, simulation of atmospheric physics and accuracy. The models are listed by name in alphabetical order.

There are three separate conditions under which these models will normally be approved for use: first, if a demonstration can be made that the model produces concentration estimates equivalent to the estimates obtained using a preferred model (e.g., the maximum or high, second-high concentration is within 2% of the estimate using the comparable preferred model); second, if a statistical performance evaluation has been conducted using measured air quality data and the results of that evaluation indicate the model in Appendix B performs better for the application than a comparable model in Appendix A; and third, if there is no preferred model for the specific application but a refined model is needed to satisfy regulatory requirements. Any one of these three separate conditions may warrant use of these models. See Section 3.2, Use of Alternative Models, for additional details.

Many of these models have been subject to a performance evaluation by comparison with observed air quality data. A summary of such comparisons for models contained in this appendix is included in "A Survey of Statistical Measures of Model Performance and Accuracy for Several Air Quality Models", EPA-450/4-83-001. Where possible, several of the models contained herein have been subjected to rigorous evaluation exercises, including (1) statistical performance measures recommended by the American Meteorological Society and (2) peer scientific reviews.

Any availability statement for models in this appendix that refers to the User's Network for Applied Modeling of Air Pollution (UNAMAP) should be ignored since the UNAMAP is no longer operational. However, a source for some of these models and user's documentation is:

Computer Products
National Technical Information Service (NTIS)
U.S. Department of Commerce

Springfield, VA 22161
Phone: (703) 487-4650

A number of the model codes and selected, abridged user's guides are also available from the Support Center for Regulatory Air Models Bulletin Board System[19] (SCRAM BBS), Telephone (919) 541-5742. The SCRAM BBS is an electronic bulletin board system designed to be user friendly and accessible from anywhere in the country. Model users with personal computers are encouraged to use the SCRAM BBS to download current model codes and text files.