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Project Summary

Livermore Regional Air Quality (LIRAQ) Model (Transfer to EPA)

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Methods were developed to convert data from the Regional Air Pollution/ Regional Air Monitoring Study (RAPS/RAMS) into a format compatible with the Livermore Regional Air Quality (LIRAQ) models. Changes made in the LIRAQ models include (1) improved map plotting routines, (2) updated chemical mechanism, and (3) a partial SO_2 oxidation mechanism. In the final report which is available from NTIS (see last page of this summary), several appendices serve as a user's guide to the LIRAQ models and the associated data conversion routines.

Introduction

The Livermore Regional Air Quality (LIRAQ) models were developed when, through the Research Applied to National Needs (RANN) program, the National Science Foundation supported a 2½-year interagency effort by the University of California Lawrence Livermore Laboratory (LLL), the Bay Area Air Pollution Control District (BAAPCD), and the NASA Ames Research Center (ARC) to develop and evaluate the LIRAQ-1 and LIRAQ-2 models. These codes are deterministic two-dimensional Eulerian grid air-quality models that compute spatial and temporal distributions of significant air pollutants from specified emissions, meteorological conditions, topography, and initial and boundary concentrations. LIRAQ-1 deals with chemical species that are not strongly affected by chemical reactions and uses a flux-corrected transport scheme. LIRAQ-2 treats chemically reactive species, but uses simple upstream differencing to treat the transport.

In 1976, LLL entered into an interagency agreement with the U.S. Environmental Protection Agency to modify and extend the LIRAQ models to include sulfur species (SO_2 and sulfates) and to prepare data processors for the necessary input files to be developed from EPA Regional Air Monitoring Study (RAMS) data tapes so that the LIRAQ models could participate in the Regional Air Pollution Study (RAPS). The improved codes are designated LIRAQ-1S and LIRAQ-2S.

The present EPA-supported interagency effort consists of a limited program intended to facilitate the examination of LIRAQ performance as part of RAPS. This effort included only minimal model development; the bulk of the effort was spent to develop data preprocessors and operating procedures for use by remote users of LIRAQ on the Lawrence Berkeley Laboratory (LBL) computer system.

A temporary emissions inventory was provided by the EPA late in 1978. As a result, less effort than was intended has been devoted to model verification and the analysis of poorly known but important model inputs such as specification of upper and upwind boundary conditions, and an estimate of the

reliability of the procedures used in estimating mixing depths. As yet, no final emissions inventory has been established and no model tuning has been attempted. A limited set of sensitivity studies have been carried out, but are not described in this document since no funding exists to analyze the results.

Conclusions

Under an interagency agreement with the EPA, LLL has modified the LIRAQ models for participation in the Regional Air Pollution Study (RAPS). The modification to the LIRAQ models have included:

1. Modifications to the chemical mechanism in LIRAQ-2S, so that the model now includes a representation of the homogenous gas phase photochemistry for conversion of SO_2 and $SO_4^=$, and an update of the reaction rates and mechanisms to reflect the data available in March 1976.
2. Several input checks (in both models) to ensure that all input files (source, meteorology, and initial condition) refer to the same day.
3. Changes in the topographic input designed to improve the versatility of river and coastline-plotting routines.

In addition, LLL has:

1. Developed processors that generate LIRAQ input files from RAPS data tapes.
2. Converted MASCON and VERF processors to standard FORTRAN and exported them to Lawrence Berkeley Laboratory (LBL).
3. Provided documentation.

Because LLL has not yet been provided with an emission inventory considered reliable by the EPA, little can be said about how reliable or suitable our estimates are for initial conditions, boundary conditions, or mixing depths.

Sensitivity experiments for St. Louis concentrations indicate that model predictions for O_3 are sensitive to the upper boundary condition. There are almost no data in the standard RAPS data base that can be used to guide the choice of upper boundary conditions, although pertinent data were taken in some of the special studies sponsored by RAPS. Unless data from the special studies are used, pollutant concentrations aloft will provide a set of poorly known parameters capable of strongly influencing model predictions. The treatment of such factors will be a central issue in questions of verification and in future applications of complex models such as control-strategy evaluation. At present, there is no adequate basis for judging LIRAQ performance.

Of the changes made in LIRAQ for RAPS, the update of the chemical mechanism and changes in the treatment of the steady-state species for LIRAQ-2S, the consistency checks added to the input, and the transfer of VERF and MASCON codes to LBL, all are likely to be immediately used by other LIRAQ users. The addition of $SO_2/SO_4^=$ chemistry seems less likely to be useful.

Recommended future changes in LIRAQ include a further updating of model chemistry, removal of SO_2, $SO_4^=$, and HNO_3 from LIRAQ-2S, and the addition of peroxyacylnitrates, a simplification of LIRAQ-2S numerics, and possibly an expansion of the LIRAQ-2S grid. These changes should result in either a material decrease in running time or an increase in spatial resolution.

The LIRAQ model makes the assumption that the dispersion, transport, and transformation of pollutants can be represented by treating only a single atmospheric layer extending from the surface to the normal temperature inversion. This assumption, coupled with the assumed behavior of pollutant concentration in the vertical, will be most valid when:

1. Pollutants are emitted primarily at the surface or below the inversion (the single-layer model does not keep track of pollutants emitted above the inversion).
2. Vertical dispersion is limited by a strong and persistent inversion.
3. Vertical mixing in the layer is rapid compared with horizontal transport across a grid cell.
4. Pollutant concentrations in the layer result primarily from emissions within the layer rather than prescribed fluxes through the inversion.

Application of the LIRAQ model to St. Louis, rather than the typical west-coast-maritime, inland-valley regime for which it was designed, strains the condition of the single-layer assumption. Many emission sources, particularly for SO_2, are elevated point sources that persist in the inversion and then may be mixed to the surface as the inversion rises, a process LIRAQ does not treat. The atmospheric structure in St. Louis often involves multiple, weak or nonexisting inversions creating layers that are alternately coupled and isolated during a diurnal cycle, a process crudely treated in LIRAQ. Vertical mixing can be rapid during daylight hours, but is often weak, thus the height of mixing (or single-layer depth) is not always well-defined. The elevated emissions and the multiple stable layers coupled with the diurnal cycle mean that pollutant concentrations in the single layer may often be strongly influenced by pollutants not emitted in that layer. Taken together, the characteristics of LIRAQ and St. Louis indicate that expectations of good verification should not be high and verification and analysis should be carefully pursued.

The preliminary results of LIRAQ simulations of O_3 in St. Louis involve substantial underprediction. This could reflect basic model error, improper boundary/initial conditions, emissions inventory errors or excessive mixing of NO_x from elevated sources down to the surface.

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The complete report, entitled "Livermore Regional Air Quality (LIRAQ) Model (Transfer to EPA)," (Order No. 80 221591; Cost: $14.00, subject to change) will be available from:

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