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STUDY TITLE: Development of the Next Generation Air Quality Models for Outer Continental Shelf (OCS) Applications.

REPORT TITLE: Development of the Next Generation Air Quality Models for Outer Continental Shelf (OCS) Applications.

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KEY WORDS: Air quality modeling; meteorology; overwater boundary layer; CALPUFF; standard meteorological dataset; modeling software.

BACKGROUND: As a result of significant advances in the scientific understanding of dispersion modeling over the last couple of decades, the MMS has identified a need to develop a model for application to emission sources on the Outer Continental Shelf (OCS) that incorporates, to the extent feasible, the most current knowledge and is versatile enough to be used in short-range as well as long-range applications. The goal of this study was to enhance an existing air quality model for applications involving overwater transport and coastal interaction effects.

OBJECTIVES: (1) To perform a comprehensive review of existing models and to evaluate their applicability to offshore applications based on current knowledge of boundary layer and atmospheric dispersion in ocean and shoreline environments; (2) To revise or enhance an existing air quality model to make it suitable for offshore and coastal applications; (3) To develop a software package that includes the needed meteorological pre-processors, meteorological model, air quality model, source codes, test cases, and user's guide; (4) To carry out sensitivity testing and evaluate model performance against available tracer data.

DESCRIPTION: The new model for OCS applications is an extensively updated version of the CALPUFF (Scire et al., 2000a, 2000b) modeling system. Individual components had been compared with other modeling approaches in OCD (DiCristofaro and Hanna, 1989), AERMOD (Cimorelli et al., 2002), and SCIPUFF (EPRI, 2000). These comparisons included the model formulation equations as well as sensitivity tests performed on individual modules (e.g., boundary layer parameters, turbulence profiles over water, plume spread formulations).

Enhancements introduced into the CALPUFF modeling system included new technical features parameterizing the overwater boundary layer and coastal effects on dispersion, ease-of-use features

in the graphical user interface and new utility programs, and a standard one-year (2003) preprocessed dataset for the Gulf of Mexico area. The performance evaluation of the new model led to the formulation of a turbulence advection mechanism in CALPUFF when it was discovered that advected turbulence is an important feature of the dispersion documented in the Oresund experiments, when releases were made at the coast during off-shore flow.

The major new features in CALMET include an option to use the Coupled Ocean Atmosphere Response Experiment (COARE) overwater flux model (Fairall et al., 2002); a convective overwater boundary layer height computed for conditions of positive surface heat flux; a new convective mixing height parameterization (Batchvarova and Gryning, 1991,1994) option; and an automatic height adjustment of surface winds from anemometer height to the middle of CALMET Layer 1.

CALPUFF has been modified to include new features for building downwash at elevated offshore platform structures with an open area between the water surface and the raised structure; an option to use AERMOD turbulence profiles; an option to accept the AERMET version of SURFACE and PROFILE meteorological data files; and an adjustment for turbulence advection from regions of larger turbulence velocity into regions of smaller turbulence velocity.

The CALPUFF graphical user interface was extensively revised and enhanced, including new processors for buoy data and NCEP model output; a new utility for extracting a user-defined subset of data from the standard 2003 Gulf of Mexico dataset; extensively revised and enhanced graphical display modules to allow animations, contour plots, vector plots and other types of graphical displays. The standard Gulf of Mexico meteorological and ozone dataset was prepared, which includes one full year (2003) of gridded prognostic meteorological output fields from the Rapid Update Cycle (RUC) mesoscale weather model covering the MMS Gulf of Mexico domain, data for 13 buoy stations, 21 upper stations, 230 hourly surface meteorological stations, 271 precipitation stations, 201 ozone monitoring stations and terrain and land use data for the modeling domain.

SIGNIFICANT CONCLUSIONS: Sensitivity tests and a model evaluation have shown that the COARE overwater flux model results in improved model performance over the OCD model and previous CALPUFF formulations. The standard COARE option performed as well with these datasets as more complex COARE options including shallow water adjustments or a wave model. A minimum value of the lateral turbulence velocity of water (0.37 m/s) different from the overland value (0.5 m/s) results in improved model performance. Turbulence advection was found to be important in a coastal application in offshore flow situations with a coastal source. AERMOD turbulence profiles performed as well or slightly better than the original turbulence-based parameterization in CALPUFF. Consideration of the convective mixing height over water was determined to provide important improvements in mixing height estimates over water. The Batchvarova-Gryning convective mixing height model showed improved performance over the Maul-Carson method in the evaluation datasets.

STUDY RESULTS: A new, technically-enhanced version of the CALPUFF modeling system has been developed and provided to the MMS. A model evaluation study with five overwater and coastal datasets has shown substantial improvement of the new model over the Offshore and Coastal Dispersion (OCD) steady-state model and previous versions of CALPUFF for these types of applications. Significant enhancements and new modules in the Graphical User Interfaces and the development of a standard modeling dataset for the year 2003 have made the modeling platform significantly easier to use.

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Standard CALMET/CALPUFF Dataset for 2003 including RUC data, surface observations, upper air observations, precipitation data, buoy data and geophysical data for the Gulf of Mexico area.

CALPUFF Modeling System including model codes, graphical user interfaces and test case datasets.

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