

MMS MODEL DEVELOPMENT STUDY

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

SAC Meeting

June 1-2, 2005

The Woodlands, Texas

Earth Tech, Inc.

196 Baker Avenue

Concord, Massachusetts 01742

Introduction

- Air Quality Model Development for Outer Continental Shelf (OCS) Applications
 - Develop a generalized regulatory model for evaluating air quality impacts from sources located on federal waters on the OCS
 - Short-range (tens of meters) and long range transport (several hundred km)
 - Offshore and coastal impacts
 - Averaging times from 1-hour to one year
 - Criteria pollutants (SO_2 , NO_x , CO, PM_{10}), toxic pollutants, sulfate and nitrate (visibility)

Study Objectives

- Review of existing puff models
- Revise and enhance existing air quality model
 - Easy of use
 - Technical Enhancements
- Conduct sensitivity testing and evaluate model performance
- Develop and package software and documentation

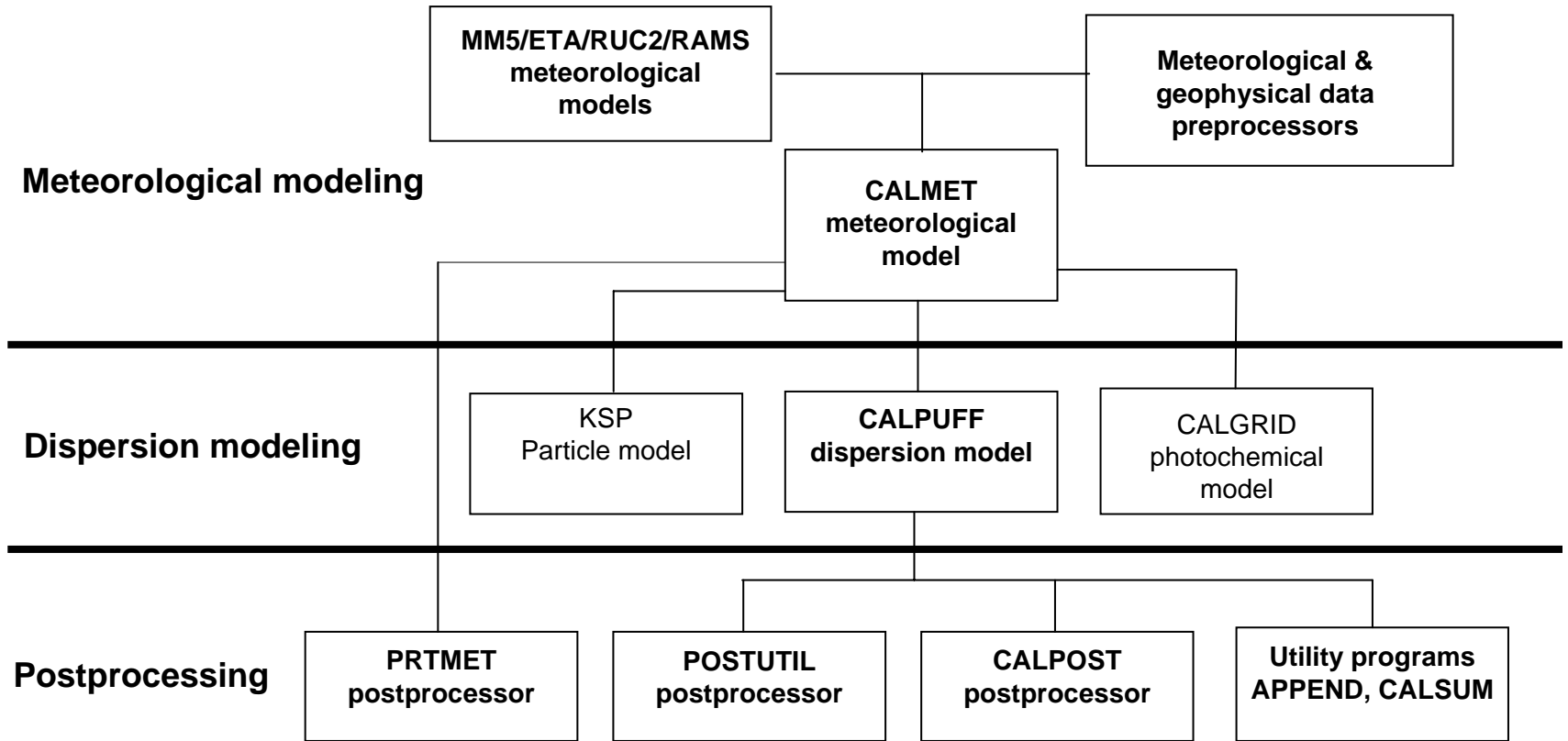
Overview

- Improvements in datasets for OCS applications
 - Enhanced interface (MM5) and new interfaces (RUC, NAM/Eta, RAMS)
 - 3d and 2d datasets
 - High resolution SST data
 - Standard 1-year MM5 meteorological dataset
- Ease-of-use enhancements
 - Graphical User Interfaces
 - Graphics – vectors, isopleths, animations
- Technical enhancements to CALPUFF modeling system
 - COARE algorithms
 - Improve mixing height algorithm over water including buoyancy effects
 - Option for AERMOD-like turbulence profiles
 - Subgrid-scale coastline treatment and TIBL growth
 - Non-Boussinesq numerical plume rise for all sources
 - Platform adjustments to building downwash algorithms

Background

- CALPUFF is a Lagrangian, non-steady-state puff dispersion model
- Achieved status as a U.S. EPA *Guideline Model* (Federal Register, 15 April 2003)
- Recommended by IWAQM (1998) for long-range transport applications
- Recommended by FLAG (2000) for Class I impact assessments and air quality related value impact evaluation

CALPUFF Modeling System



CALMET Model

- CALMET boundary layer modules
 - Computes mixing heights, surfaces fluxes, stability and turbulence fields
 - Overland PBL model uses an energy balance approach
 - Overwater PBL model uses a profile method
- CALMET 3-D diagnostic wind field module
 - Uses observations and/or gridded prognostic meteorological fields
 - Wind fields adjusted for fine-scale terrain effects and mass-consistency
 - Slope flows, kinematic effects, terrain blocking effects
 - Divergence minimization
 - Objective analysis procedure to assimilate observational data

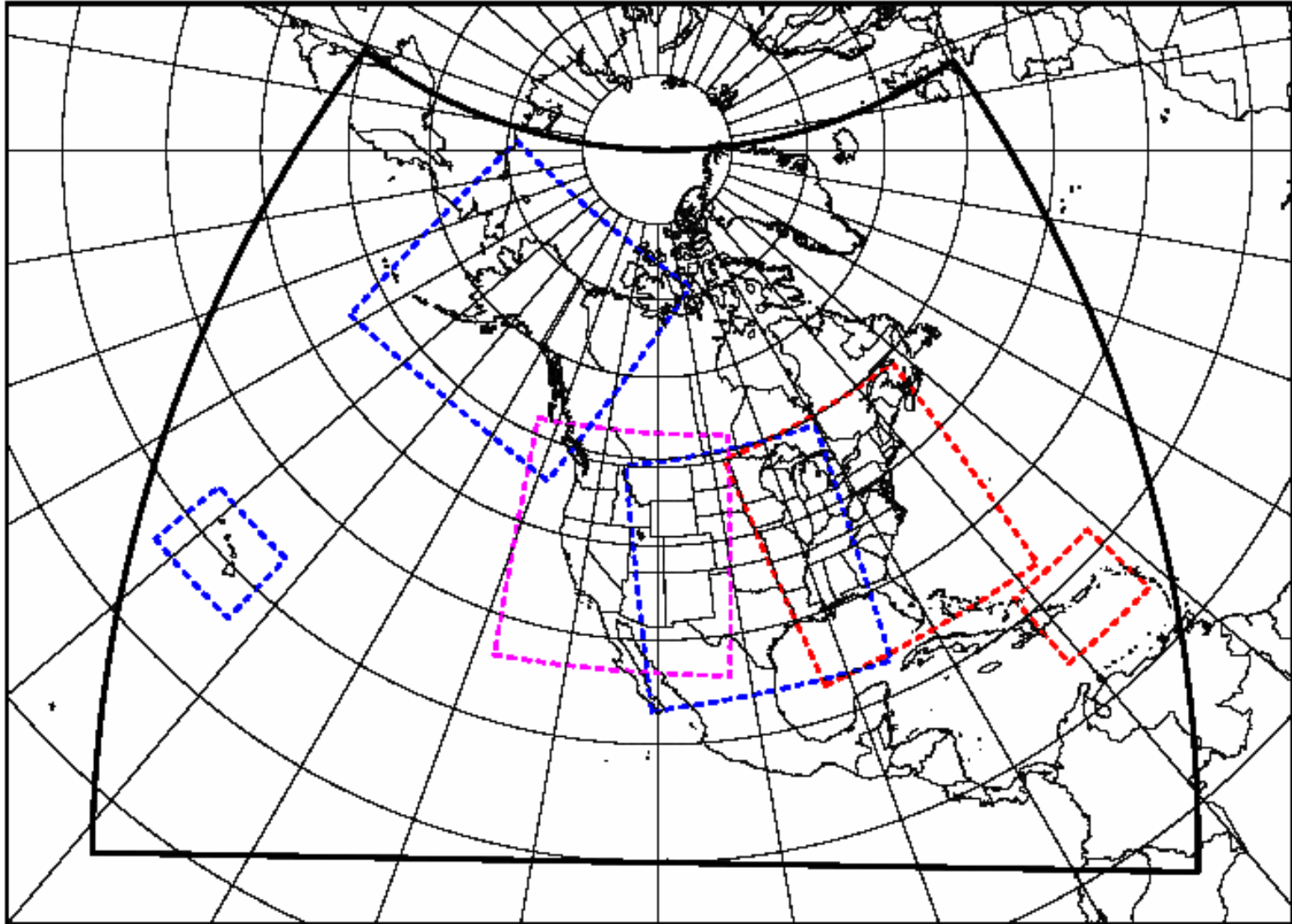
Improvements in Datasets

- High resolution satellite data in defining SST
- Prognostic model to define conditions, especially in data sparse offshore areas
- Gridded air-water temperature structure (gridded SEA.DAT file)
- Introduction of “no-observations” mode in CALMET
 - Closer coupling of CALMET with prognostic meteorological models
- New interfaces to additional prognostic models such as RUC, NAM/Eta, RAMS in addition to MM5

Standard Meteorological Dataset

- Standard dataset for regulatory applications
 - Consistency of meteorological fields across applications
 - Substantial savings of effort
 - Evaluated dataset with known performance
- MM5 dataset being developed by Penn State under separate MMS contract for the GOM area
 - One year period (Oct 1, 2000 – Sept 30, 2001)
 - Three nests: 36km, 12km and 4km nests
 - Using high resolution SST data
- Additional years with MM5 or output from other models
 - New programs developed to interface CALMET to RUC, Eta and RAMS

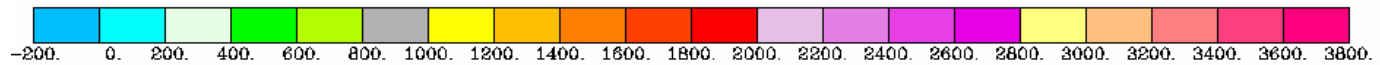
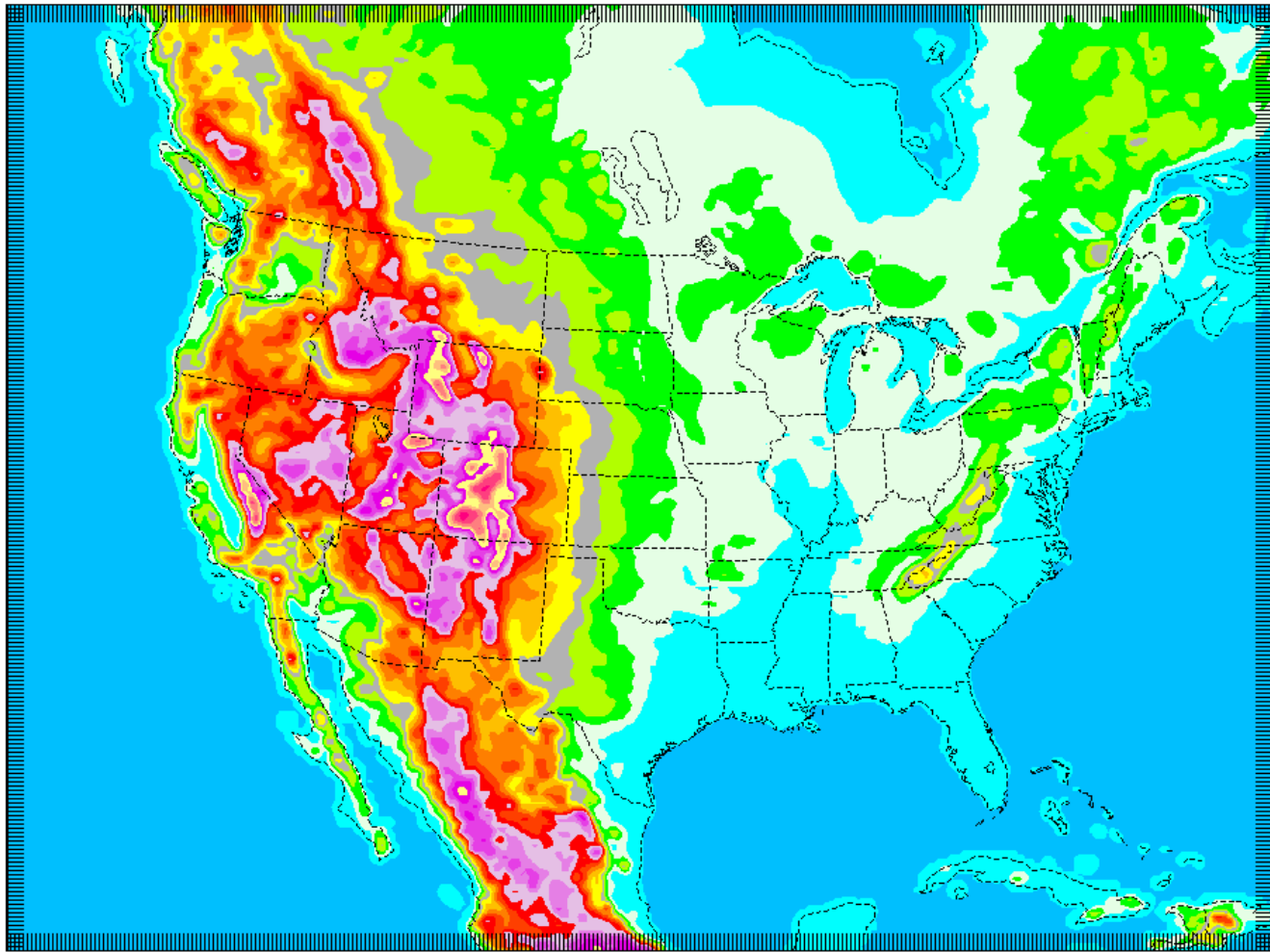
NAM (Eta) Modeling Domains



RUC Modeling Domain

20km RUC
A -

MAX= 3692.736 MIN= -1.000 INT= 200.000

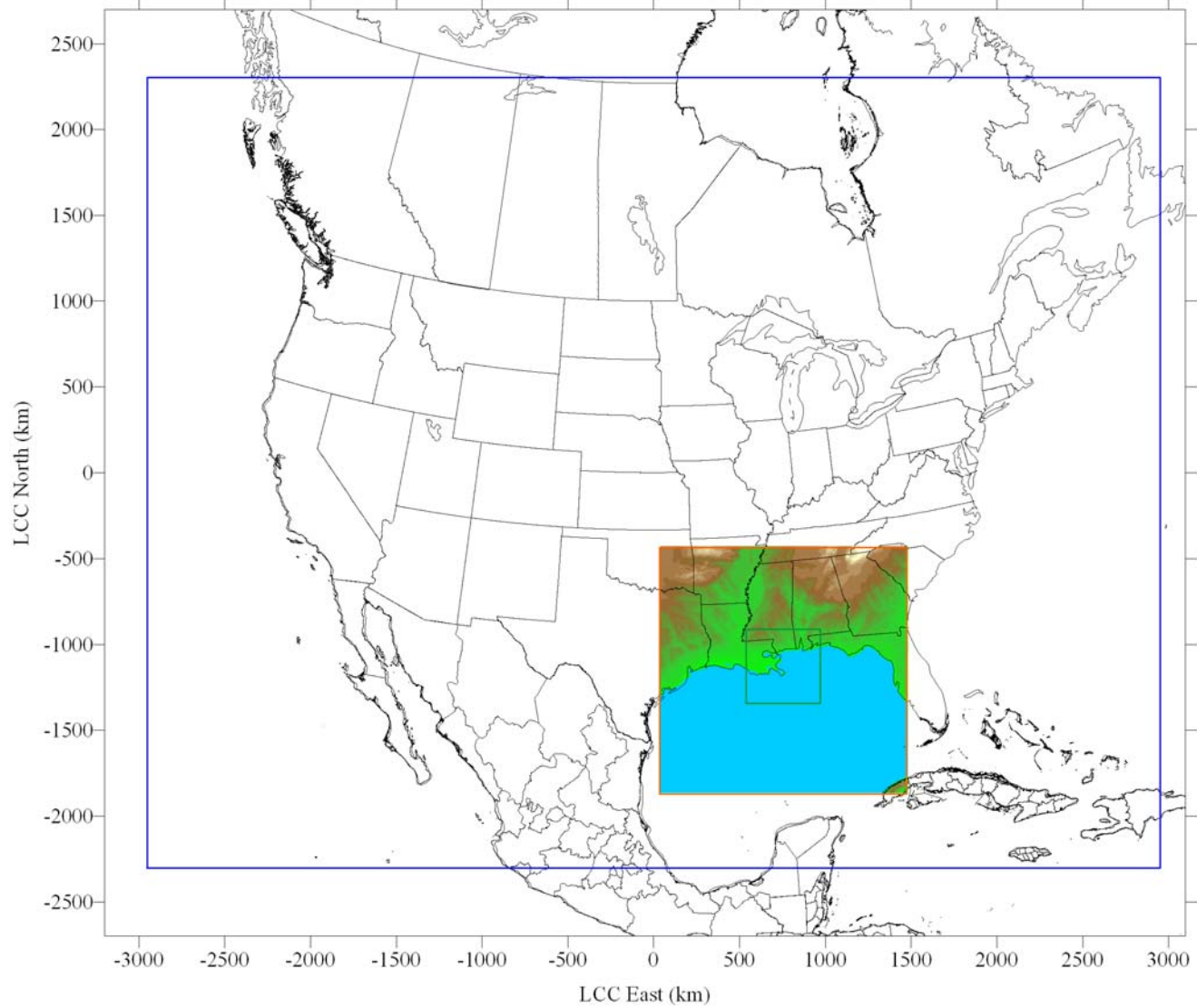


Summary of Eta/RUC Operational Runs

Model	Horizontal Resolution (km)	Vertical Resolution	Run Frequency	Output Interval		Forecast Length
				Analysis	Forecast	
ETA	12	60 Levels	4 per day	6-hours	3-hours	84 Hours
ETA	8	60 Levels	4 per day	6-hours	3-hours	48 Hours
RUC	20	50 Levels	24 per day	1-hour	1-3 hour	12-Hours

MMS

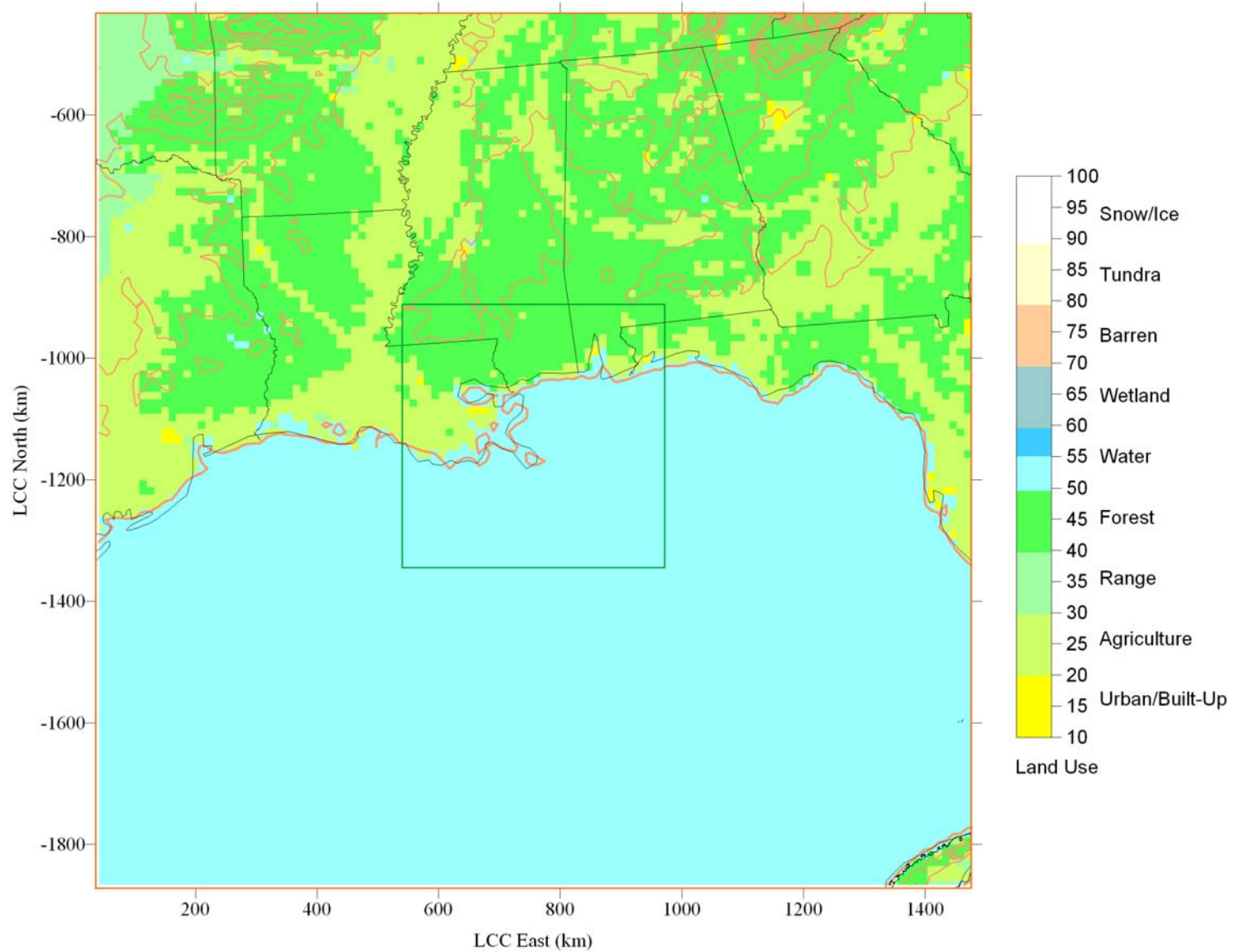
Modeling Domains



(LCC Origin Lat. = 40.0 N, Origin Lon. = 97.0 W, Parallel 1 = 33.0 N, Parallel 2 = 45.0 N, Datum = WGS-84)

MMS

Modeling Domains



(LCC Origin Lat. = 40.0 N, Origin Lon. = 97.0 W, Parallel 1 = 33.0 N, Parallel 2 = 45.0 N, Datum = WGS-84)

Satellite SST Datasets

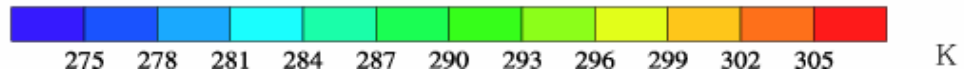
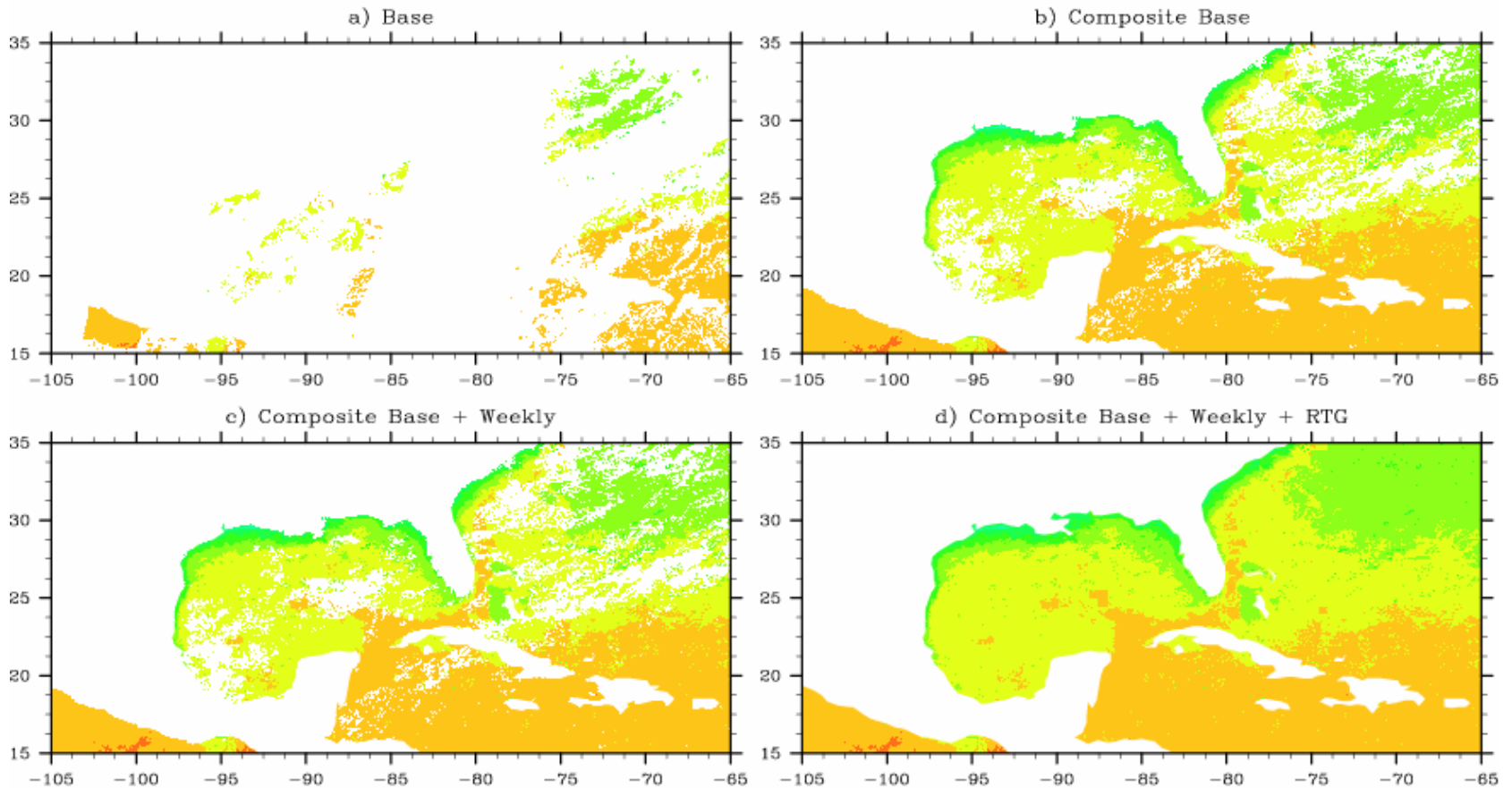
- Final Analysis Data (FNL)
 - 1 deg x 1 deg data
 - Available 4 times daily
 - Data assimilation
- Real-time, global SST Analysis (RTG)
 - 0.5 deg x 0.5 deg
 - Available daily
 - Analysis of satellite measurements, surface obs and interpolation
- Moderate Resolution Imaging Spectroradiometer (MODIS)
 - 4km data
 - Daily and weekly
 - Satellite measurements

Development of MODIS SST Dataset

- Any given satellite pass has potentially large amounts of missing data due to clouds
- Procedure being tests:
 - Base: Satellite data for Day: n
 - Composite: Fill missing cells iteratively with data for day $n+1, n-1, n+2, n-2, n+3, n-3$
 - Composite + weekly: Fill missing cells with data from weekly MODIS dataset
 - Composite + weekly + RTG: Fill any remaining missing data with daily RTG data

Illustration of Steps in Developing SST Dataset

SST Data on Jan 1, 2002



Evaluation of MM5 Performance

- Conducted by Penn State
- Initial results presented in Jan 2005 for three model configurations
 - Analysis nudging, RTG SST data
 - Observations nudging added
 - Obs nudging + 4-km MODIS SST data
- Results indicated improvements in both winds and temperature fields as obs nudging added and again when high resolution SST data added
- Evaluation is ongoing

Convective Boundary Layer

- New convective mixing height parameterization:
 - Batchvarova and Gryning (1990, 1994)
- 2 options overland:
 - Maul-Carson (original) (when positive buoyancy flux)
 - Batchvarova and Gryning (when positive buoyancy flux)
- 3 options over water:
 - Mechanical OCD always
 - Maul-Carson (original) (when positive buoyancy flux)
 - Batchvarova and Gryning (when positive buoyancy flux)
- Above convective mixing height lapse rates:
 - Land: observed (UP.DAT soundings) or prognostic (e.g. MM5)
 - Water: observed (SEA.DAT or constants) or prognostic (e.g. MM5)

New convective boundary layer input parameters

- IMIXH : convective boundary layer parameterizations
 - 1: Maul-Carson for land and water cells
 - -1: Maul-Carson for land cells only – Original OCD mixing height overwater (old CALMET)
 - 2: Batchvarova and Gryning for land and water cells
 - -2: Batchvarova and Gryning for land cells only - Original OCD mixing height overwater
- THRESHW: threshold buoyancy energy flux per meter of marine boundary layer required for boundary layer growth over water (default: $0.05 \text{ W/m}^2 /\text{m}$)
- THRESHL: threshold buoyancy energy flux per meter of land boundary layer required for boundary layer growth over land (default: $0.05 \text{ W/m}^2 /\text{m}$)
- ITWPROG: overwater lapse rates above the current OW mixing height
 - 0 : use SEA.DAT air/sea temperatures and lapse rates for the marine BL growth
 - 1 : use SEA.DAT air/sea temperatures and MM5 lapse rates

CALPUFF UPGRADES

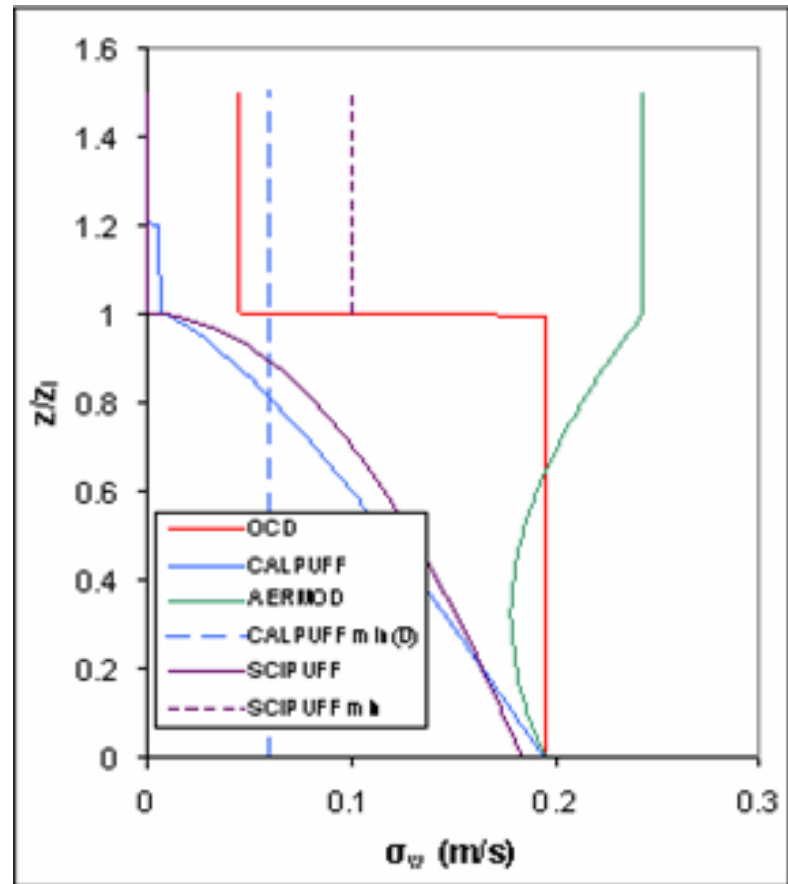
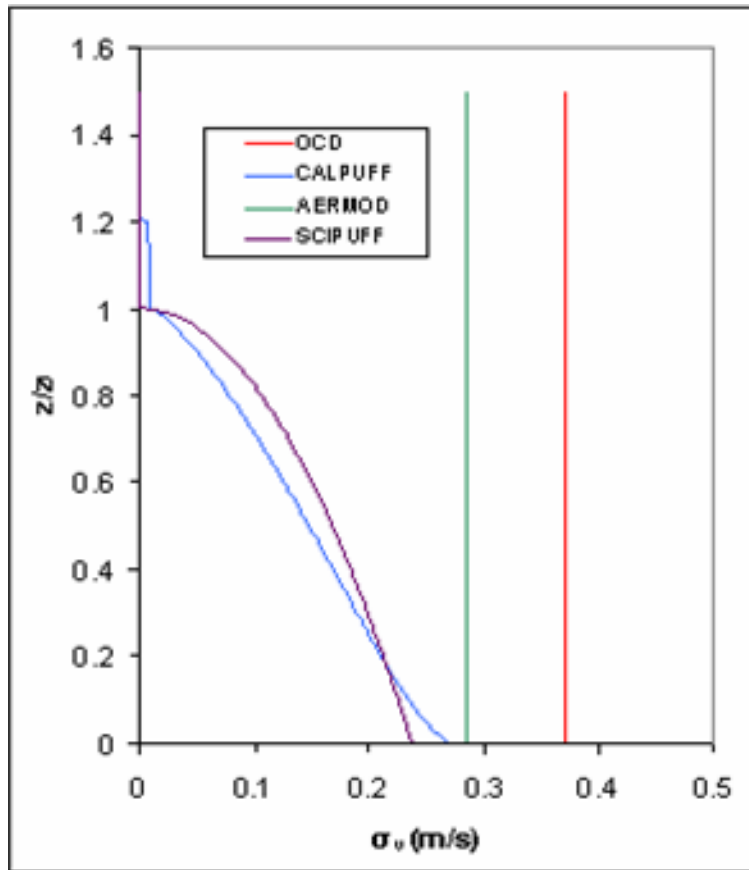
- Building downwash adjustment for elevated (platform) structures with an open area between the surface and the bulk of the structures. Currently implemented for ISC downwash.
- Option for computing gridded turbulence profiles using the AERMOD subroutines.
- Option to specify Lagrangian time-scale for lateral plume growth functions
- AERMET version of SURFACE and PROFILE met data files
- Numerical plume rise for hot plumes (e.g., flares)

AERMOD Turbulence Option

- Compared OCD, CALPUFF, SCIPUFF and AERMOD algorithms for computing profiles of sigma-v and sigma-w from surface layer parameters
 - CALPUFF and SCIPUFF include similar vertical structure within the surface layer; AERMOD and OCD use constant sigma-v(z)
 - AERMOD includes a residual sigma-w aloft for the stable BL
 - Include option for AERMOD profiles
- New control file variable to allow switching of turbulence schemes from standard CALPUFF scheme to AERMOD scheme
 - Method used to compute turbulence sigma-v & sigma-w using micrometeorological variables (MCTURB)
 - 1 = Standard CALPUFF subroutines
 - 2 = AERMOD subroutines

AERMOD Turbulence Option

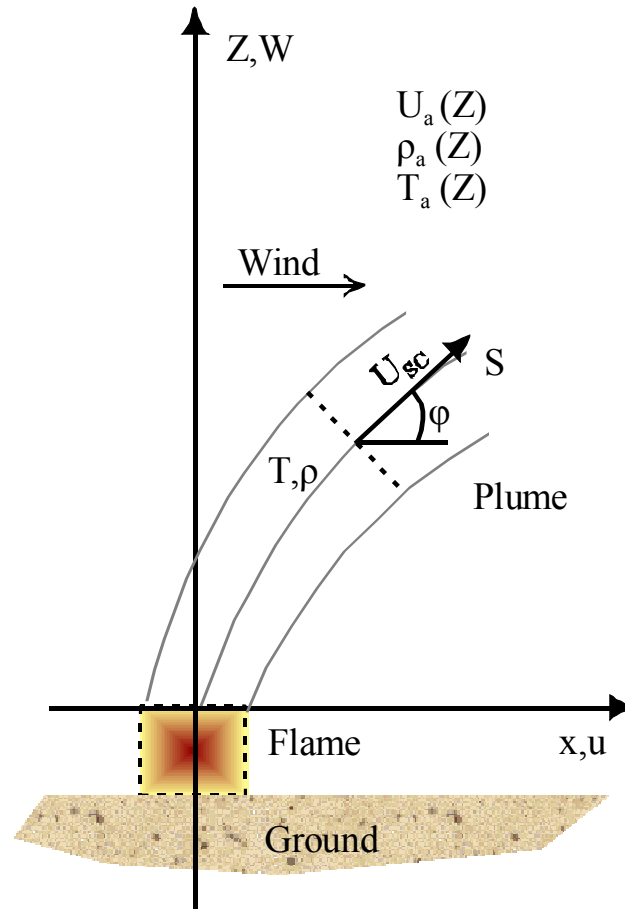
(Example for $L=50$ m, $u_{\text{star}}=0.15$ m/s)



Numerical Plume Rise

- Numerical solution to conservation and state equations in non-Boussinesq form (used for high temperature sources such as flares or fires)
- Initial properties at release
 - temperature
 - effective vertical velocity
 - effective radius
- Explicitly accounts for vertical structure of atmosphere
 - wind speed profile
 - wind direction profile
 - temperature (density) profile

SCHEMATIC FOR A PLUME IN A CROSSWIND



Numerical Plume Rise Conservation Eqns

- Mass

$$\frac{d}{ds}(\rho u_{sc} r^2) = 2r\alpha\rho_a |u_{sc} - u_a \cos\phi| + 2r\beta\rho_a |u_a \sin\phi|$$

- Momentum - along-wind

$$\frac{d}{ds}(\rho u_{sc} r^2 (u - u_z)) = -r^2 \rho_w \frac{du_a}{dz}$$

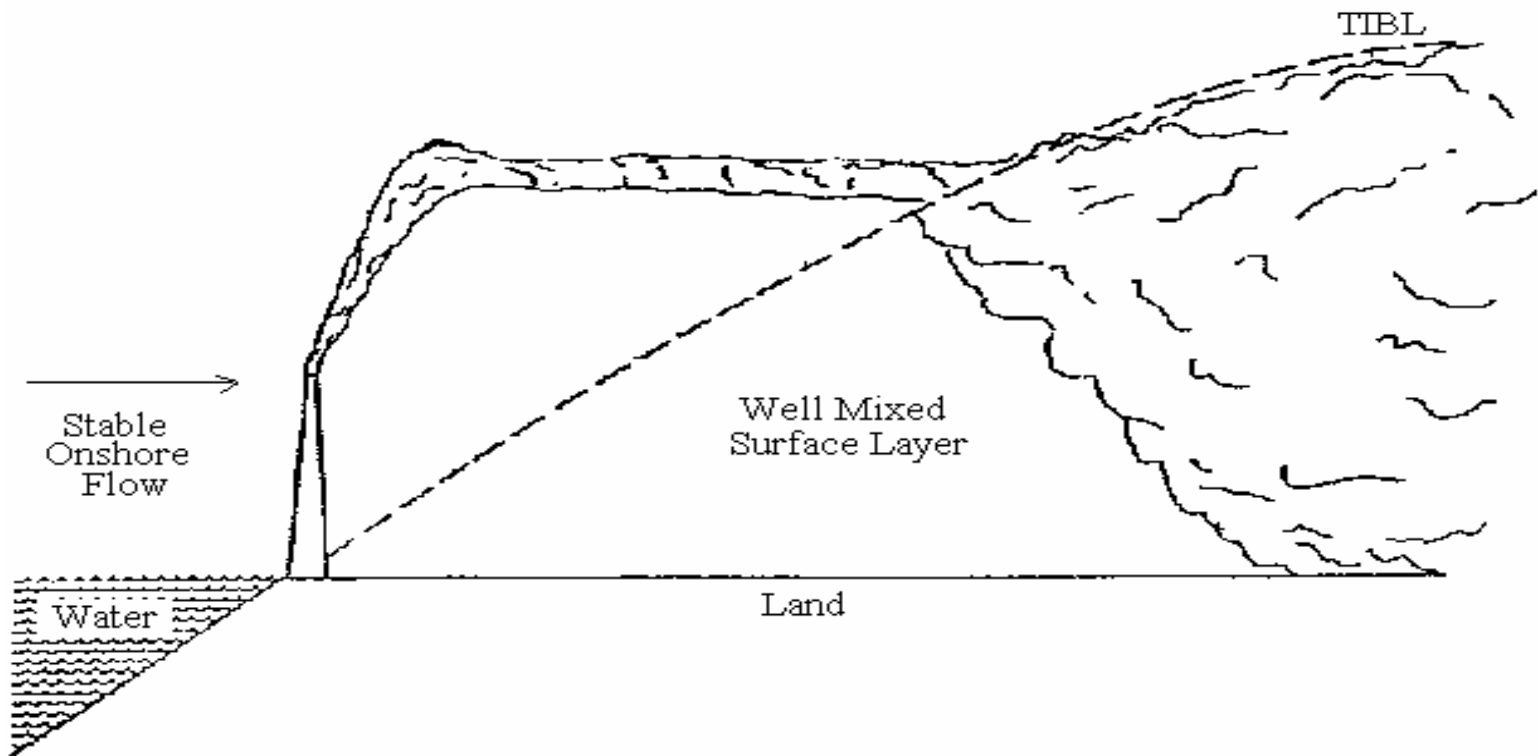
- Momentum – vertical

$$\frac{d}{ds}(\rho u_{sc} r^2 w) = g r^2 (\rho_a - \rho)$$

- Energy

$$\frac{d}{ds}[\rho u_{sc} r^2 (T - T_a)] = -\left(\frac{dT_a}{dz} + \frac{g}{c_p}\right) \rho_w r^2 - R_p r (T^4 - T_a^4)$$

Plume Fumigation



TIBL

- OCD
 - Piece-wise linear mixed layer height is prescribed along the direction from the source to a receptor with distance measured from the coast
 - $h = 0.1 x$ for $x \leq 2000\text{m}$
 - $h = 200 + 0.03 (x-2000)$ for $x \geq 2000\text{m}$
 - Designed to approximate a generic TIBL without inputs for wind speed, heat flux, marine layer lapse rate

TIBL

- CALMET
 - 2-Step mixing height procedure
 - (1) Gridded mixing height field computed using local grid-cell properties
 - (2) Advective averaging scheme controlled by user inputs smoothes transitions by averaging heights along flow
 - Provides robust treatment of coastal-zone transitions, recognizing difference in along-shore / on-shore / off-shore situations

TIBL

- CALPUFF

- Sub-grid TIBL option refines the gridded mixing height structure in coastal zones using the TIBL model of Garrett (1992)

$$\frac{dh}{dx} = \frac{(1 + 2\beta)H}{\gamma\rho c_p u h}$$

- Model is applied along the puff trajectory using local grid cell properties.
- For steady conditions,

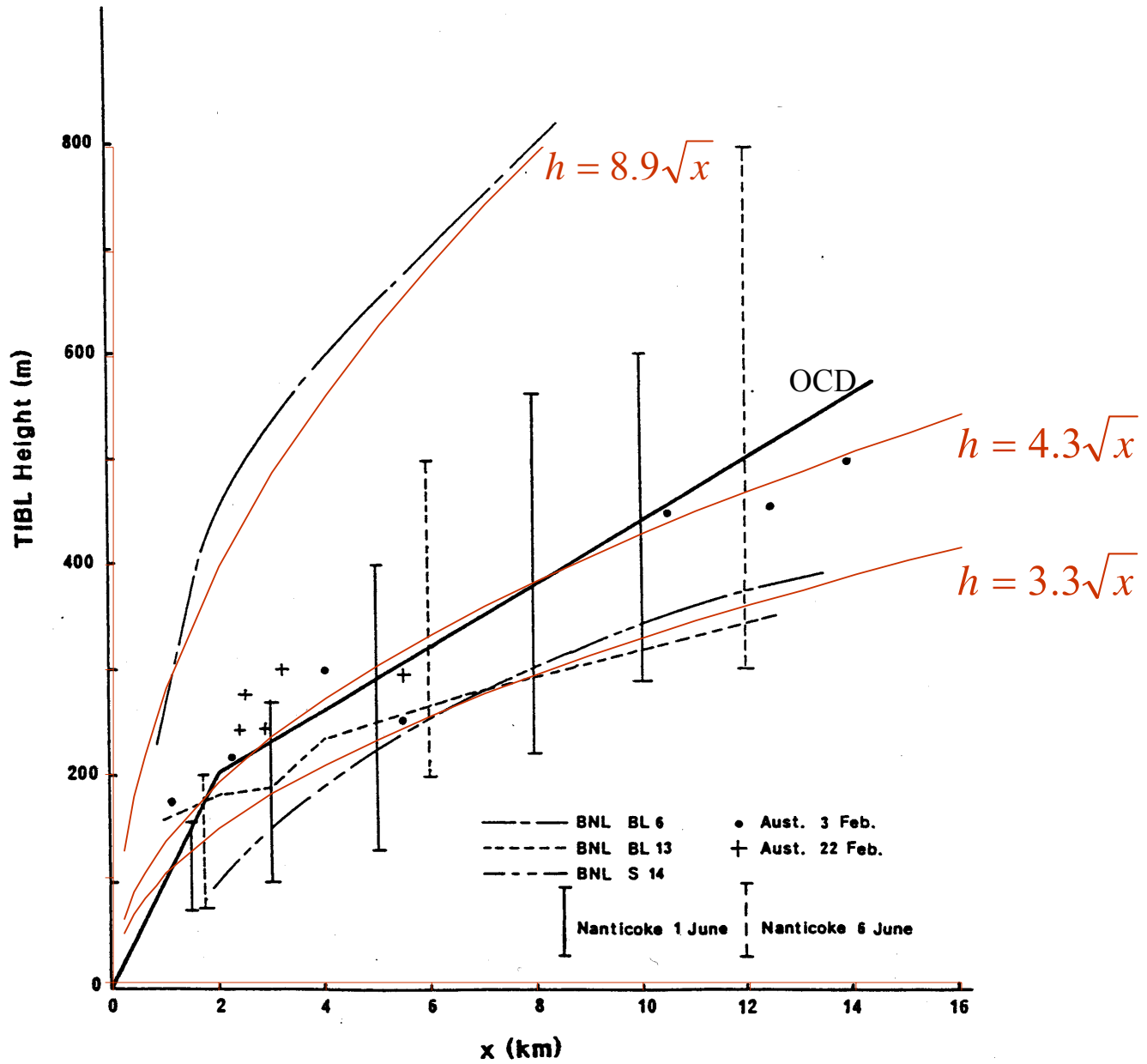
$$h = \sqrt{\frac{2(1 + 2\beta)H}{\gamma\rho c_p u} x}$$

TIBL

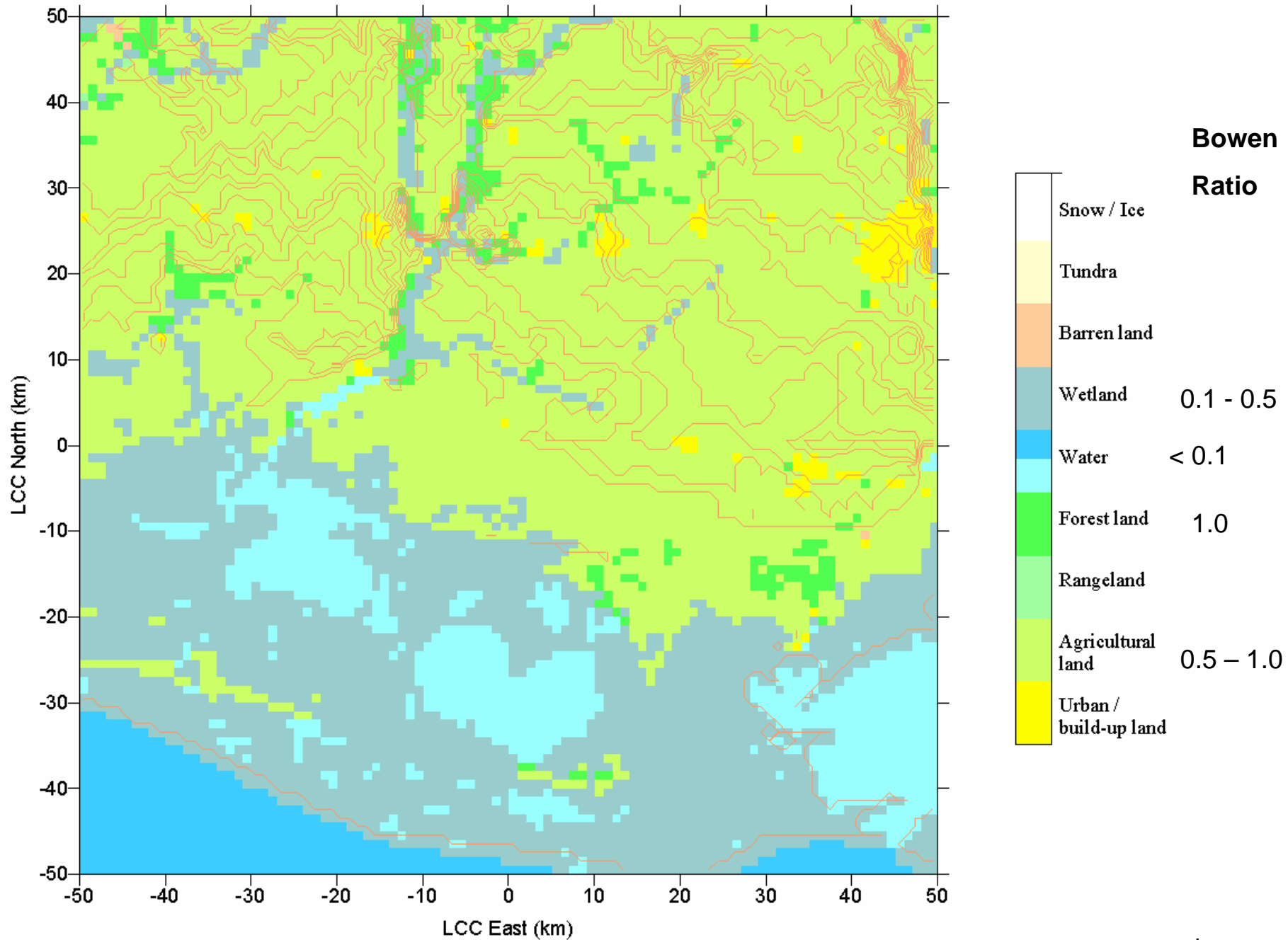
- CALPUFF (Coastal Zone Representation)
 - Gridded land use includes wetlands and inland water bodies
 - Properties tied to land use includes roughness length and Bowen Ratio
 - Sensible heat flux (H) is proportional to Bowen Ratio
 - Computed TIBL growth rate will respond to coastal zone properties:

$$\frac{dh}{dx} = \frac{(1 + 2\beta)H}{\gamma\rho c_p u h}$$

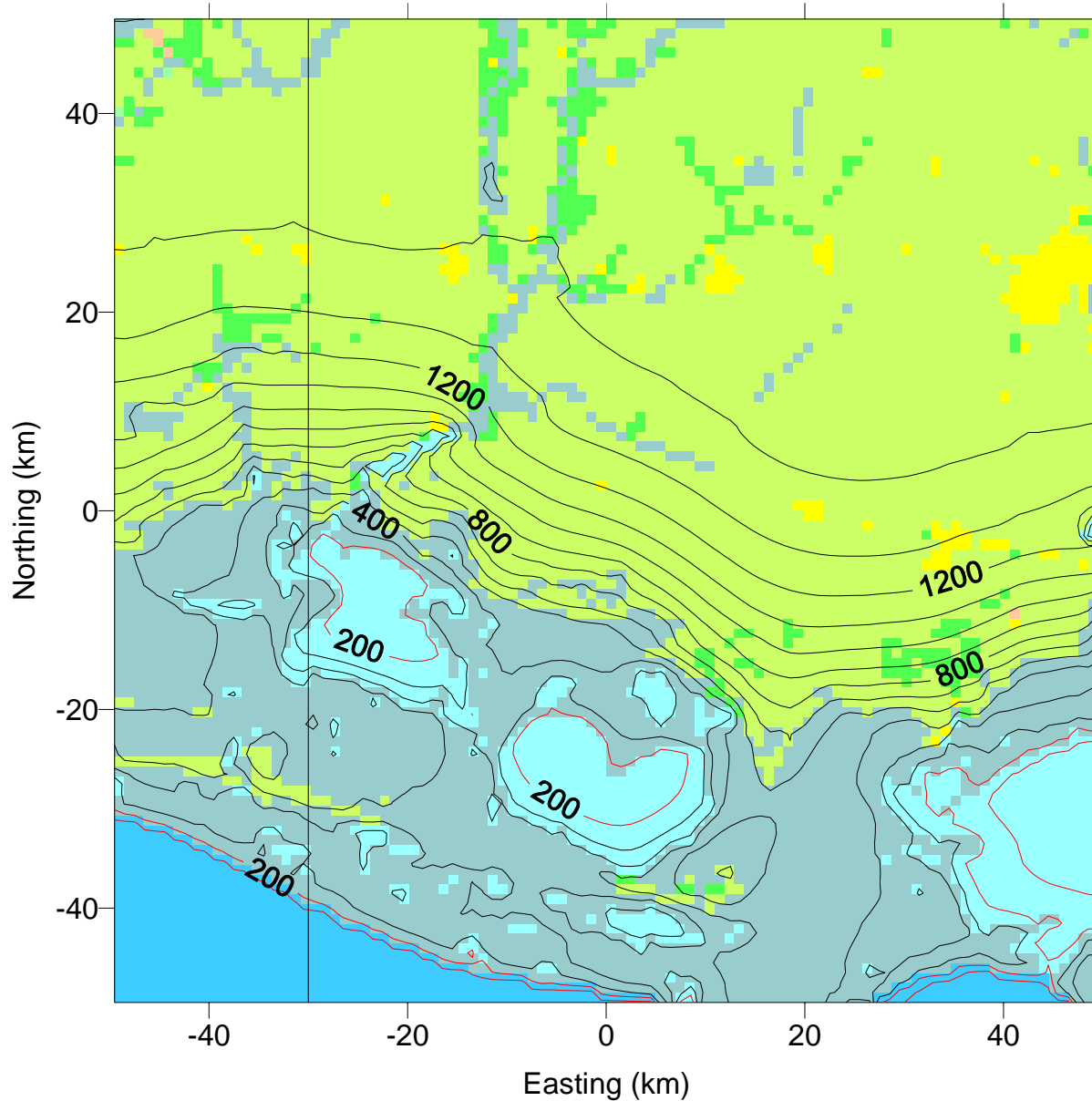
OCD TIBL Comparison with Field Data



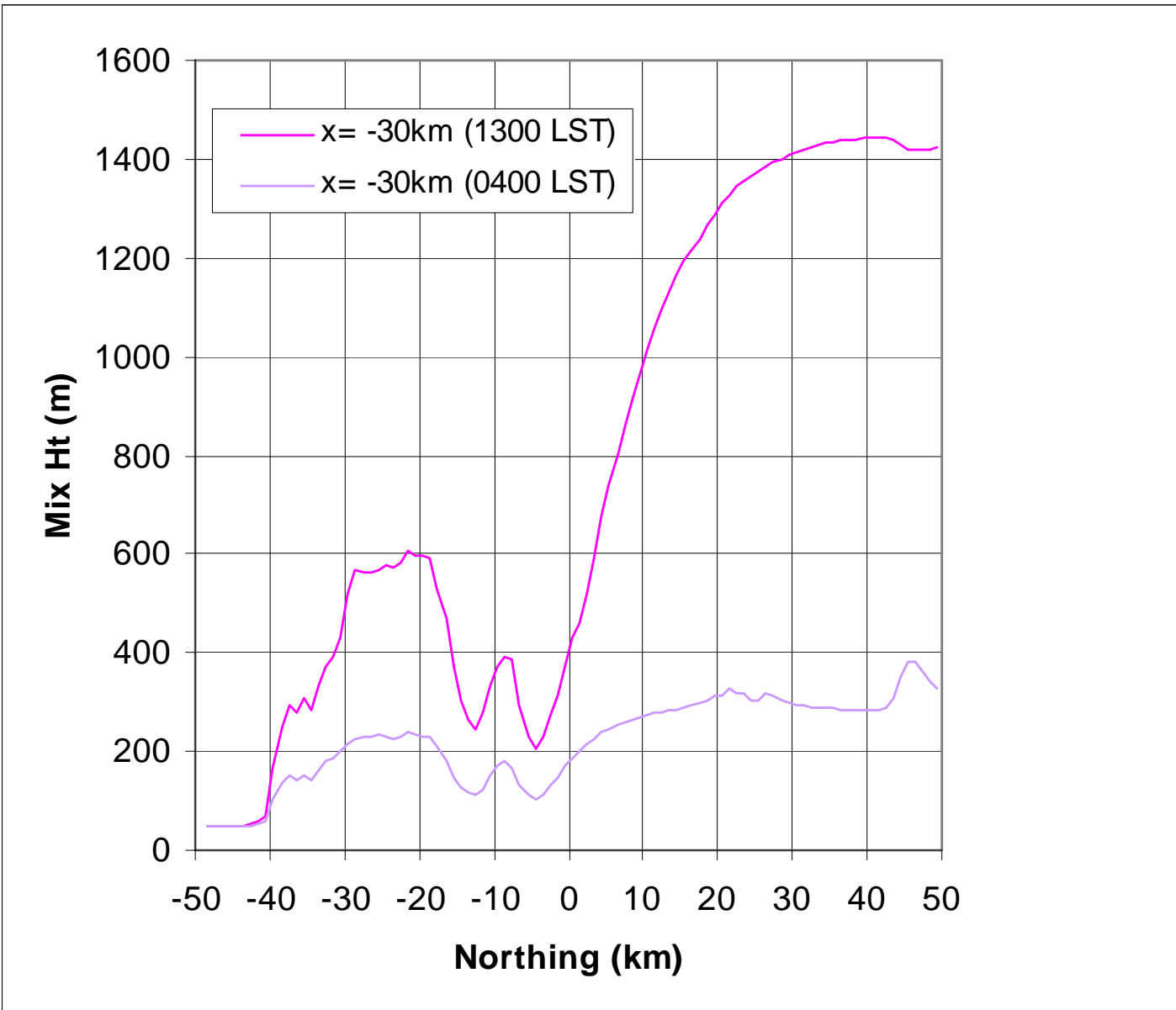
Land Use and Terrain in Lake Charles, LA area



Computed Mixing Heights (m) 1300 LST



Mixing Heights along $X=-30\text{km}$



Conclusions

- Improvements made in datasets for OCS applications
 - Use of prognostic datasets important in data sparse areas offshore
 - Enhancements to allow better use of prognostic meteorological datasets
 - Addition of new interfaces to allow new options for data sources (MM5 + RUC, Eta, RAMS)
 - High resolution SST data developed based on MODIS 4km data
 - Standard 1-year MM5 meteorological dataset to be prepared for regulatory use
- Enhancements made to facilitate use of CALPUFF for regulatory applications
- Technical enhancements to CALPUFF modeling system
 - COARE algorithms
 - Improve mixing height algorithm over water including buoyancy effects
 - Option for AERMOD-like turbulence profiles
 - Subgrid-scale coastline treatment and TIBL growth
 - Non-Boussinesq numerical plume rise for all sources
 - Platform adjustments to building downwash algorithms

End