Evaluation of Enhancements to the CALPUFF Model for Offshore and Coastal Applications

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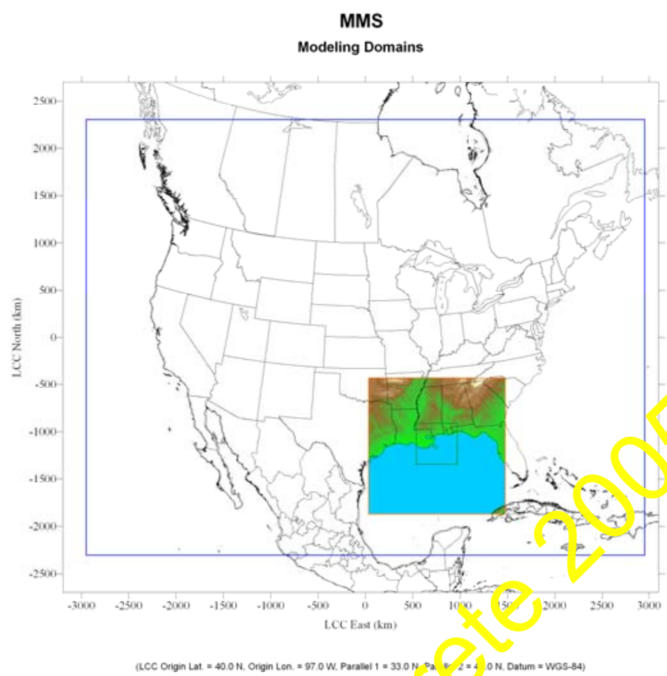
Outline of Presentation

- Overview
- Model Enhancements
- Model Evaluation
- Summary and Conclusions

Overview

- MMS in charge of development of mineral resources in Outer Continental Shelf (OCS) of the USA
- Offshore and Coastal Dispersion (OCD) steady-state model currently used for regulatory applications from sources on the OCS
- Objective: optimize the non-steady-state CALPUFF model for regulatory use for OCS sources
  - Short-range and long range transport
  - Offshore and coastal impacts
  - Averaging times from 1-hour to one year
  - Criteria pollutants (SO_2, NO_x, CO, PM_{10}), toxics



Model Enhancements - CALMET

- CALMET is a diagnostic meteorological model
- Use of COARE[1] overwater flux model
- Improvement in mixing height algorithms
  - Consider convective mixing heights over water
  - Testing of Maul-Carson (M-C) scheme and Batchvarova-Gryning (B-G) scheme (1994)
- Subgrid-scale coastal boundary and Thermal Internal Boundary Layer (TIBL) growth
- Development of a standard meteorological dataset for Gulf of Mexico area
  - New interfaces to MM5, RAMS, RUC and Eta/NAM models
  - Rapid Update Cycle (RUC) data from NCEP initialization fields
  - High resolution sea surface temperature (SST) data

[1] Coupled Ocean Atmosphere Response Experiment

Model Enhancements - CALPUFF

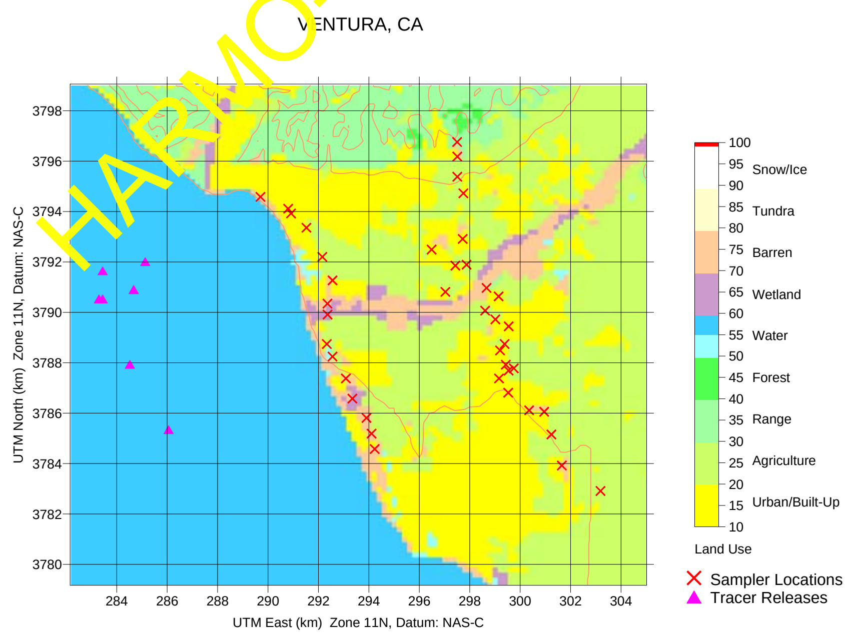
- Non-steady-state Lagrangian puff model
- Advection of turbulence, e.g., from overland to overwater
- Minimum lateral turbulence velocity (σ_v) – 0.5 m/s (land) and 0.37 m/s water
- Compute turbulence profiles using AERMOD algorithms
- Adjustments for elevated structures (platform downwash)
- Draxler (1976) vs SCIPUFF Lagrangian time scale for lateral plume growth

Evaluation Datasets

- OCD datasets
  - Ventura, Carpinteria, Pismo Beach, Cameron
  - Gaviota (not used in OCD4 evaluations; deferred due to ½-hour timesteps)
  - Major test feature of all datasets is overwater dispersion over 4-8km range except for Carpinteria and Gaviota (<1km), both stable and unstable
  - Travel time to samplers can be substantial fraction of hour (hourly met data and sampler data not aligned at times)
- Oresund Experiment
  - Tracer experiments across 20km-wide strait of Oresund between Denmark and Sweden

Ventura, CA

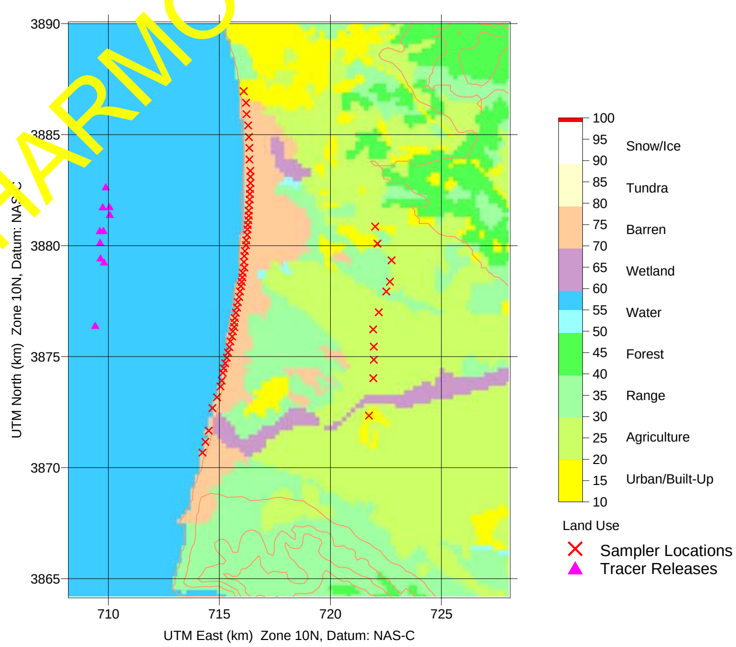
Period	SEP 24,27,28,29 - 1980 (“Fall”) - afternoon JAN 6,9,13 - 1981 (“Winter”) - afternoon
Tracer	SF_6
Source	8.1m MSL from boat 5-7 km from shore Boat downwash H=7m, L=20m
Sampling	Arc1: near the shoreline (within 500m) Arc2: about 7 km inland
Met Data	Boat: Wind speed and Sigma-Theta at 20.5m, T(air) at 7m, T(sea) Aircraft: T(z)
Averaging time	1 hour
Comment	Overwater boundary layer unstable in Fall, stable in Winter Wind speed averaged about 4.5 m/s



Pismo Beach, CA

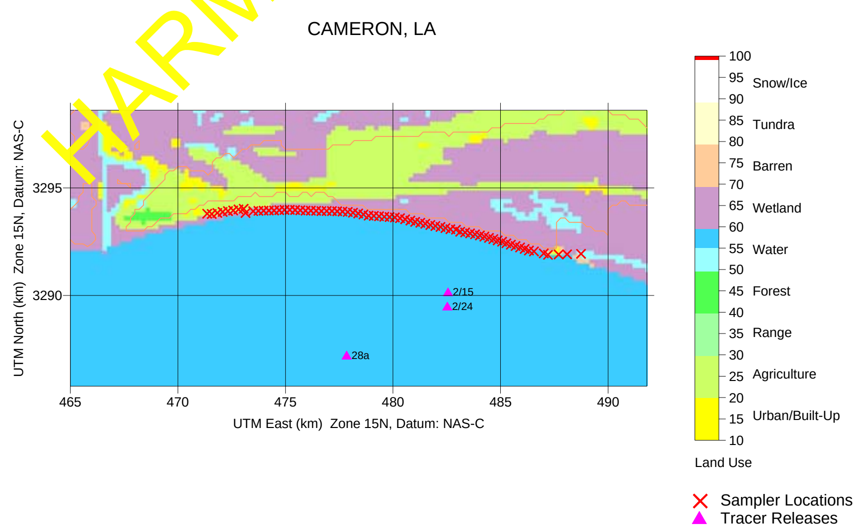
Period	DEC 8,11,13,14,15- 1981 ("Winter") - afternoon JUN 21,22,24,25,27 - 1982 ("Summer") - afternoon
Tracer	SF_6
Source	13.1m MSL from R/V Arcania 6-8 km from shore Boat downwash H=7m, L=20m
Sampling	Arc1: shoreline Arc2: about 7 km inland
Met Data	Boat: Wind speed and Sigma-Theta at 20.5m, T(air) at 7m, T(sea) Aircraft: T(z)
Averaging time	1 hour
Comment	Overwater boundary layer moderately stable for most of Winter, quite stable in Summer Wind speed averaged about 5 m/s

Pismo Beach, CA



Cameron, LA

Period	JUL 20,23,27,29 - 1981 (“Summer”) - afternoon/evening FEB 15,17,22,23,24 - 1982 (“Winter”) - afternoon
Tracer	SF_6
Source	13m MSL from Chevron Platform 28A, 6.8 km from shore 13m MSL boat mast, 4 km from shore on 2/15 and 2/24 Boat downwash H=7m, L=20m
Sampling	Shoreline
Met Data	Platform: Wind speed at 18m, T(air) at 10m, T(sea) Shoreline tower: Wind speed, Sigma-Theta, T(air) at 10m (this T(air) used in 1981 experiments) Aircraft: T(z)
Averaging time	1 hour
Comment	Overwater boundary layer neutral to stable in Winter, unstable in Summer Wind speed typically 3-5 m/s

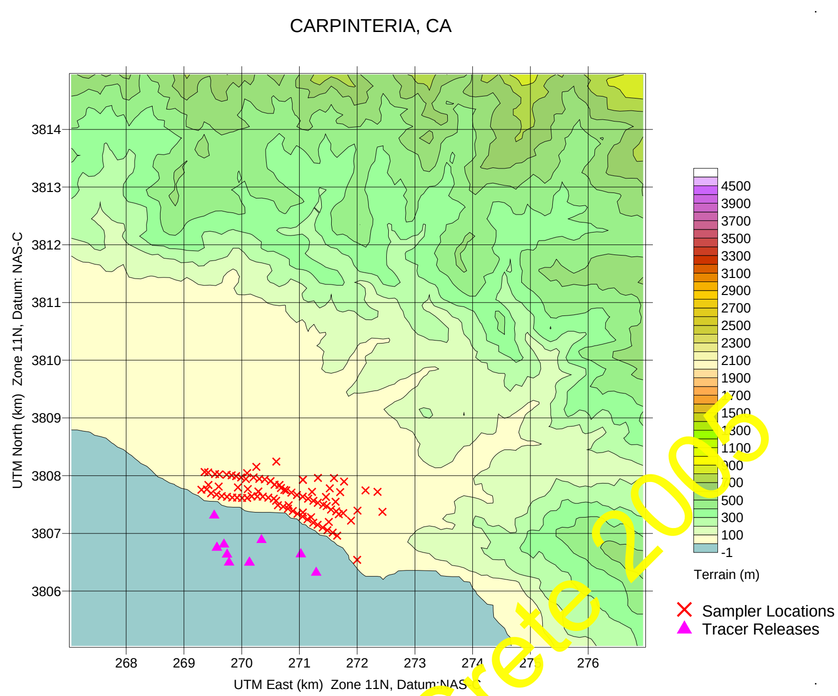


Carpinteria, CA: Terrain Study

Period	SEP 19,22,25,28,29 - 1985 (“SF_6”) - midday SEP 22,26,28,29 - 1985 (“CF_3Br”) - midday
Tracer	SF_6, CF_3Br
Source	SF_6: 18-49m MSL from boat, about ½ km from shore CF_3Br: 24-61m MSL from boat, about ½ km from shore
Sampling	Eastern grid, 30-50m shoreline bluff Arc1: shoreline bluff Arc2: about ½ km inland Arc3: about 1 km inland (sparse)
Met Data	Platform: T(air) at 9m, T(sea) Boat Tethersonde: Wind speed, Sigma-Theta at 24-49m Aircraft: T(z)
Averaging time	1 hour
Comment	Wide range in overwater stability Median wind speed 1.7 m/s

Carpinteria, CA: Fumigation Study

Period	OCT 1,3,4,5 - 1985 (“Fumigation”) - morning
Tracer	SF_6
Source	64-91m MSL from boat, about ½ km from shore
Sampling	Western grid, somewhat less terrain Arc1: shoreline bluff Arc2: about ½ km inland
Met Data	Platform: T(air) at 9m, T(sea) Boat Tethersonde: Wind speed, Sigma-Theta at 61-91m Aircraft: T(z)
Averaging time	½ hour
Comment	Wide range in overwater stability Median wind speed 1.7 m/s

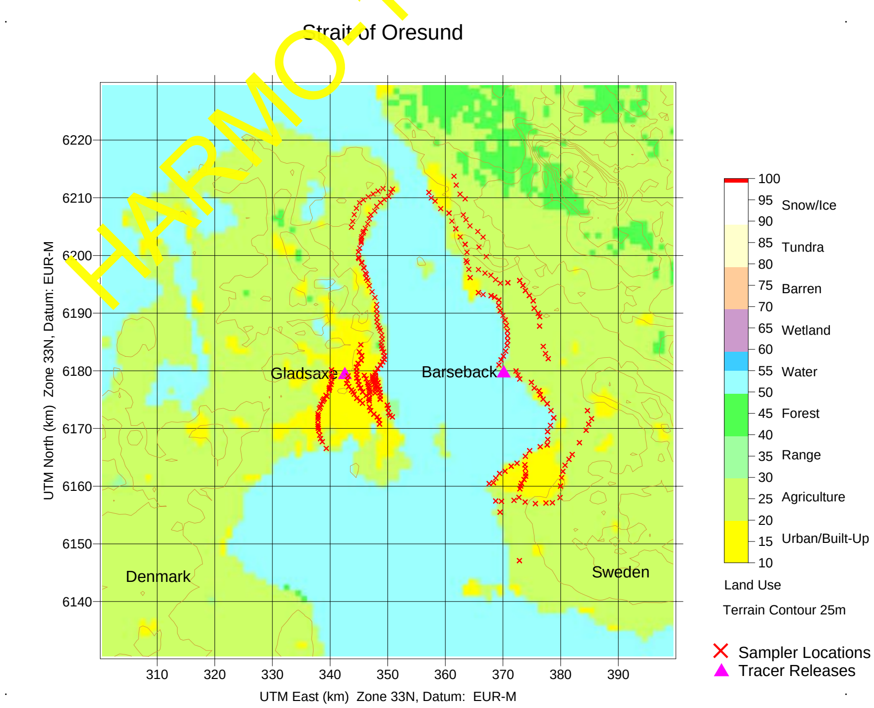


Evaluation Datasets

- Oresund Experiment
  - Tracer experiments across 20km-wide strait of Oresund between Denmark and Sweden
  - Study emphasis is “cold water” transitions with releases from Gladsaxe, Denmark or Barseback, Sweden
  - Transport distances 22-42 km to sampler arcs
  - 4 to 5 hour release from mid-morning to noon/early afternoon, with 1-hour sampling at end
  - Past analyses focus on internal BL growth (downwind land) and flow speedup over water

Strait of Oresund (Denmark/Sweden)

Period	MAY 16,18,22,29,30 - 1984 JUN 4,5,12,14 - 1984
Tracer	SF_6
Source	115m AGL (160m MSL) Gladsaxe, Denmark (3 days) 95m AGL (100m MSL) Barseback, Sweden (6 days) 4 to 5 hours / day
Sampling	1 to 4 arcs at opposite shore of Oresund
Met Data	T(air),T(sea) at Oskarsgrundet NE Lighthouse 3-hr radiosondes (1 Denmark, 1 Sweden) T(z) minisondes over Oresund (2-4 during experiments) Wind(profile) SODARS (4) 95m met tower at Barseback release WS, WD, T, RH, radiation at numerous surface stations
Averaging time	Single 1-hour sampling period/day Met data at 5-10-20-60 minutes (varies with type)



Evaluation Statistics

- Normalized peak concentrations ($C=\chi/Q$) paired in time
- Geometric mean (MG) and geometric variance (VG) give equal weight to over and underpredictions (e.g., C_o/C_p = ½ and 2)
- Perfect model MG = 1.0
- Factor of 2 scatter is VG ~ 1.6 (for no bias)
- Minimum (lnVG) = $(\ln MG)^2$

Model Option Variations

- CALMET
  - COARE/OCD overwater fluxes
  - Mixing height algorithm (B-G, C-M)
- CALPUFF
  - Measured/modeled I_y
  - Minimum sigma-v (0.5 or 0.37 m/s)
  - SCIPUFF-like computed F_y Lagrangian timescale
  - CALPUFF/AERMOD turbulence profiles
  - Terrain adjustment option

Cameron, Carpinteria, Pismo Beach, Ventura
All CALPUFF Configurations with min. Sigma-v: 0.37 m/s

CALPUFF Configuration

(Modeled Sigma-v ≥ 0.37 m/s)

A -- Modeled Iy, CALPUFF Turbs, Draxler Fy

B -- Observed Iy, CALPUFF Turbs, Draxler Fy

E -- Modeled Iy, AERMOD Turbs, Draxler Fy

F -- Observed Iy, AERMOD Turbs, Draxler Fy

C -- Modeled Iy, CALPUFF Turbs, Variable TLy

D -- Observed Iy, CALPUFF Turbs, Variable TLy

G -- Modeled Iy, AERMOD Turbs, Variable TLy

H -- Observed Iy, AERMOD Turbs, Variable Tly

CALMET Configuration

c0 – OCD overwater BL parameter module

c10d – COARE module (standard "deep water")

c10s – COARE module with shallow water adj.

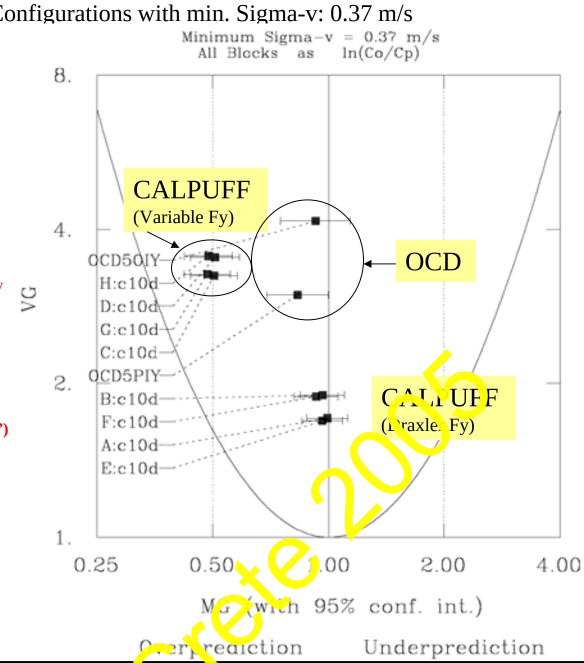
c11 – COARE module with wave option 1

c12 – COARE module with wave option 2

OCD5 Configuration

OCD5PIY - Modeled Iy (Sigma-v ≥ 0.37 m/s)

OCD5OIY - Observed Iy



Results (OCD4 Datasets)

- CALMET with standard COARE flux model options and CALPUFF with minimum sigma-v = 0.37 m/s as in OCD
  - Computed Lagrangian timescale for lateral dispersion produces a statistically significant factor of 2 overprediction; runs with standard Draxler Fy curves produce small overprediction bias that is not statistically different from zero (MG=1)
  - Using modeled Iy in CALPUFF produces less scatter and slightly fewer overpredictions than using the observed Iy
  - CALPUFF results show less scatter than OCD5, and less tendency to overpredict with standard Draxler Fy curves
  - CALPUFF/AERMOD turbulence profile choice produces similar results, with the AERMOD choice being slightly more conservative

Cameron, Carpinteria, Pismo Beach, Ventura

All CALPUFF Configurations with min. Sigma-v: 0.50 m/s

CALPUFF Configuration

(Modeled Sigma-v ≥ 0.50 m/s)

A -- Modeled Iy, CALPUFF Turbs, Draxler Fy

B -- Observed Iy, CALPUFF Turbs, Draxler Fy

E -- Modeled Iy, AERMOD Turbs, Draxler Fy

F -- Observed Iy, AERMOD Turbs, Draxler Fy

C -- Modeled Iy, CALPUFF Turbs, Variable TLy

D -- Observed Iy, CALPUFF Turbs, Variable TLy

G -- Modeled Iy, AERMOD Turbs, Variable TLy

H -- Observed Iy, AERMOD Turbs, Variable Tly

CALMET Configuration

c0 – OCD overwater BL parameter module

c10d – COARE module (standard "deep water")

c10s – COARE module with shallow water adj.

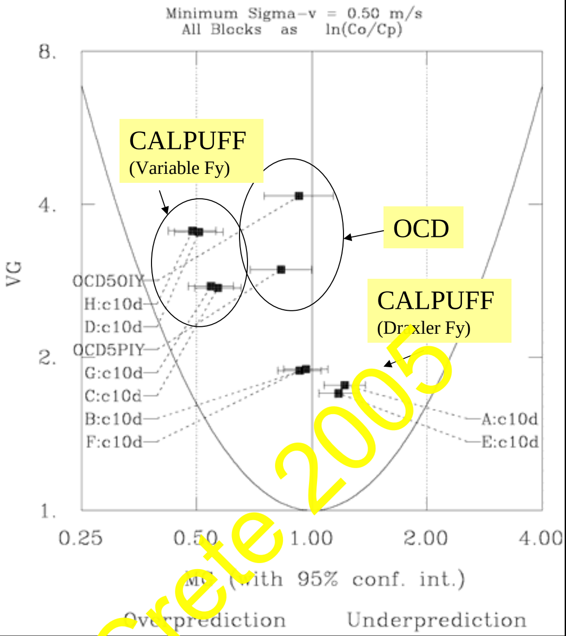
c11 – COARE module with wave option 1

c12 – COARE module with wave option 2

OCD5 Configuration

OCD5PIY - Modeled Iy (Sigma-v ≥ 0.37 m/s)

OCD5OIY - Observed Iy



Results (OCD4 Datasets)

- CALMET with standard COARE flux model options and CALPUFF with minimum sigma-v = 0.50 m/s
  - Using modeled Iy in CALPUFF with the larger minimum reduces the bias and produces a statistically significant underprediction (MG>1) with the Draxler Fy curves
  - Computed Lagrangian timescale for lateral dispersion produces a statistically significant overprediction
  - CALPUFF/AERMOD turbulence profile choice produces similar results, with the AERMOD choice being slightly more conservative

Cameron, Carpinteria, Pismo Beach, Ventura
All CALMET Configurations with CALPUFF Configuration A

CALPUFF Configuration

(Modeled Sigma-v ≥ 0.37 m/s)

A -- Modeled Iy, CALPUFF Turbs, Draxler Fy

B -- Observed Iy, CALPUFF Turbs, Draxler Fy

E -- Modeled Iy, AERMOD Turbs, Draxler Fy

F -- Observed Iy, AERMOD Turbs, Draxler Fy

C -- Modeled Iy, CALPUFF Turbs, Variable TLy

D -- Observed Iy, CALPUFF Turbs, Variable TLy

G -- Modeled Iy, AERMOD Turbs, Variable TLy

H -- Observed Iy, AERMOD Turbs, Variable Tly

CALMET Configuration

c0 – OCD overwater BL parameter module

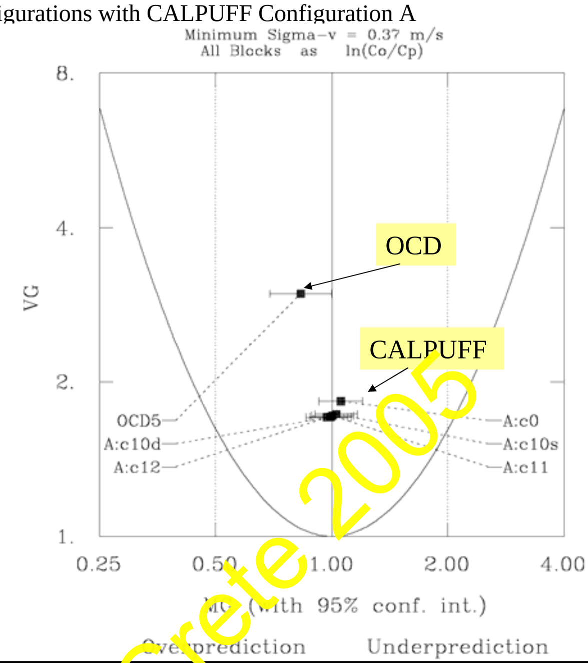
c10d – COARE module (standard "deep water")

c10s – COARE module with shallow water adj.

c11 – COARE module with wave option 1

c12 – COARE module with wave option 2

OCD5 with Modeled Iy (Sigma-v ≥ 0.37 m/s)



Cameron, Carpinteria, Pismo Beach, Ventura
All CALMET Configurations with CALPUFF Configuration B

CALPUFF Configuration

(Modeled Sigma-v ≥ 0.37 m/s)

A -- Modeled Iy, CALPUFF Turbs, Draxler Fy

B -- Observed Iy, CALPUFF Turbs, Draxler Fy

E -- Modeled Iy, AERMOD Turbs, Draxler Fy

F -- Observed Iy, AERMOD Turbs, Draxler Fy

C -- Modeled Iy, CALPUFF Turbs, Variable TLy

D -- Observed Iy, CALPUFF Turbs, Variable TLy

G -- Modeled Iy, AERMOD Turbs, Variable TLy

H -- Observed Iy, AERMOD Turbs, Variable Tly

CALMET Configuration

c0 – OCD overwater BL parameter module

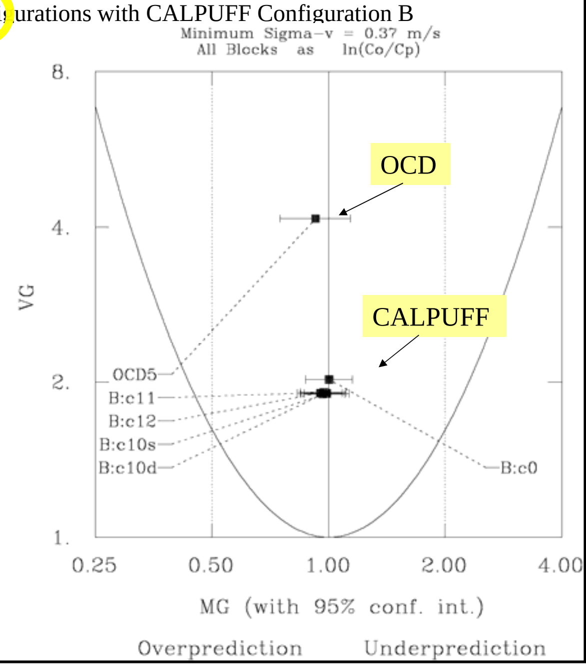
c10d – COARE module (standard "deep water")

c10s – COARE module with shallow water adj.

c11 – COARE module with wave option 1

c12 – COARE module with wave option 2

OCD5 with Observed Iy

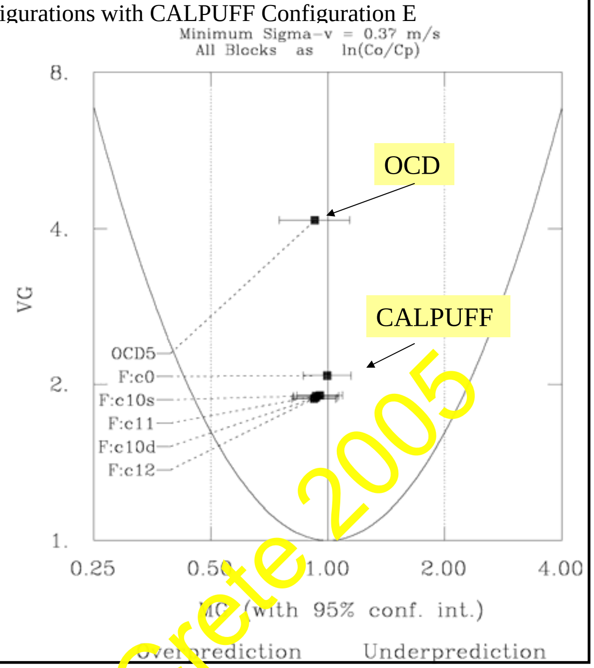


Cameron, Carpinteria, Pismo Beach, Ventura
All CALMET Configurations with CALPUFF Configuration E

CALPUFF Configuration
(Modeled Sigma-v ≥ 0.37 m/s)
A -- Modeled Iy, CALPUFF Turbs, Draxler Fy
B -- Observed Iy, CALPUFF Turbs, Draxler Fy
E -- Modeled Iy, AERMOD Turbs, Draxler Fy
F -- Observed Iy, AERMOD Turbs, Draxler Fy
C -- Modeled Iy, CALPUFF Turbs, Variable TLy
D -- Observed Iy, CALPUFF Turbs, Variable TLy
G -- Modeled Iy, AERMOD Turbs, Variable TLy
H -- Observed Iy, AERMOD Turbs, Variable Tly

CALMET Configuration
c0 – OCD overwater BL parameter module
c10d – COARE module (standard "deep water")
c10s – COARE module with shallow water adj.
c11 – COARE module with wave option 1
c12 – COARE module with wave option 2

OCD5 with Modeled Iy (Sigma-v ≥ 0.37 m/s)

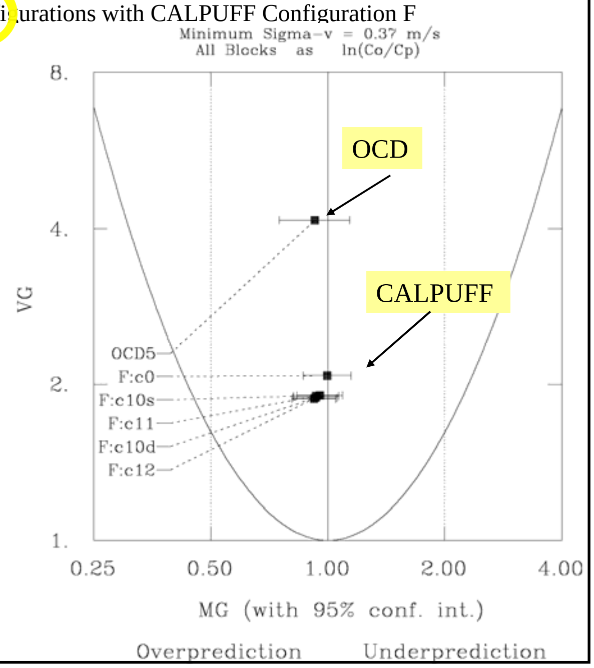


Cameron, Carpinteria, Pismo Beach, Ventura
All CALMET Configurations with CALPUFF Configuration F

CALPUFF Configuration
(Modeled Sigma-v ≥ 0.37 m/s)
A -- Modeled Iy, CALPUFF Turbs, Draxler Fy
B -- Observed Iy, CALPUFF Turbs, Draxler Fy
E -- Modeled Iy, AERMOD Turbs, Draxler Fy
F -- Observed Iy, AERMOD Turbs, Draxler Fy
C -- Modeled Iy, CALPUFF Turbs, Variable TLy
D -- Observed Iy, CALPUFF Turbs, Variable TLy
G -- Modeled Iy, AERMOD Turbs, Variable TLy
H -- Observed Iy, AERMOD Turbs, Variable Tly

CALMET Configuration
c0 – OCD overwater BL parameter module
c10d – COARE module (standard "deep water")
c10s – COARE module with shallow water adj.
c11 – COARE module with wave option 1
c12 – COARE module with wave option 2

OCD5 with Observed Iy



Results (OCD Datasets)

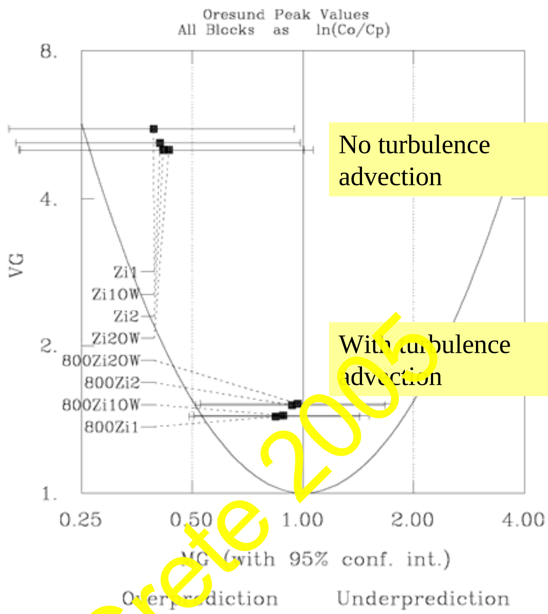
- CALMET with all COARE flux model options and CALPUFF with minimum sigma-v = 0.37 m/s as in OCD and Draxler Fy curves
  - COARE "0" option (OCD-based overwater flux model) tends to produce more scatter and a mean bias toward underprediction (although not significantly different from zero) with modeled Iy
  - COARE variations 10d, 10s, 11, and 12 result in small performance differences, with the shallow-water adjustment 10s usually associated with smaller bias
  - The standard COARE option 10d and the two wave model options 11 and 12 do not have a significantly different VG, and the MG for option 10d produces a consistently small overprediction bias

Factor of 2 and Correlation statistics

Modeled Iy	**Fraction within factor of 2**	**Correlation**
CALPUFF (CALPUFF Turbulence Profile)	0.66	0.84
CALPUFF (AERMOD Turbulence Profile)	0.67	0.85
OCD5	0.54	0.71
Observed Iy	**Fraction within factor of 2**	**Correlation**
CALPUFF (CALPUFF Turbulence Profile)	0.60	0.83
CALPUFF (AERMOD Turbulence Profile)	0.62	0.84
OCD5	0.54	0.66

Oresund

CALMET - CALPUFF Configuration
-Zi1 – No Turb Advection, Maul-Carson Mixing Ht
-Zi1OW – No Turb Advection, Maul-Carson Mixing Ht , Obs Overwater
-Zi2 – No Turb Advection, Batchvarova-Gryning Mixing Ht
-Zi1OW – No Turb Advection, Batchvarova-Gryning Mixing Ht , Obs Overwater
-800Zi1 –Turb Advection (800s), Maul-Carson Mixing Ht
-800Zi1OW –Turb Advection (800s), Maul-Carson Mixing Ht , Obs Overwater
-800Zi2 –Turb Advection (800s), Batchvarova-Gryning Mixing Ht
-800Zi1OW –Turb Advection (800s), Batchvarova-Gryning Mixing Ht , Obs Overwater



Summary and Conclusions

- CALPUFF performance produces better variance statistics than OCD and somewhat better mean values.
- Turbulence advection is an important enhancement in CALPUFF in land-to-marine BL transition.
- The COARE overwater flux module should be selected in place of the previous OCD-based model.
- The standard COARE option (no shallow water adjustment or wave model option) appears suitable to these coastal datasets, and there is little performance sensitivity among these options.
- Minimum sigma-v for overwater cells should be introduced to CALPUFF, so that a smaller minimum appropriate to overwater dispersion (e.g. 0.37 m/s) can be applied.

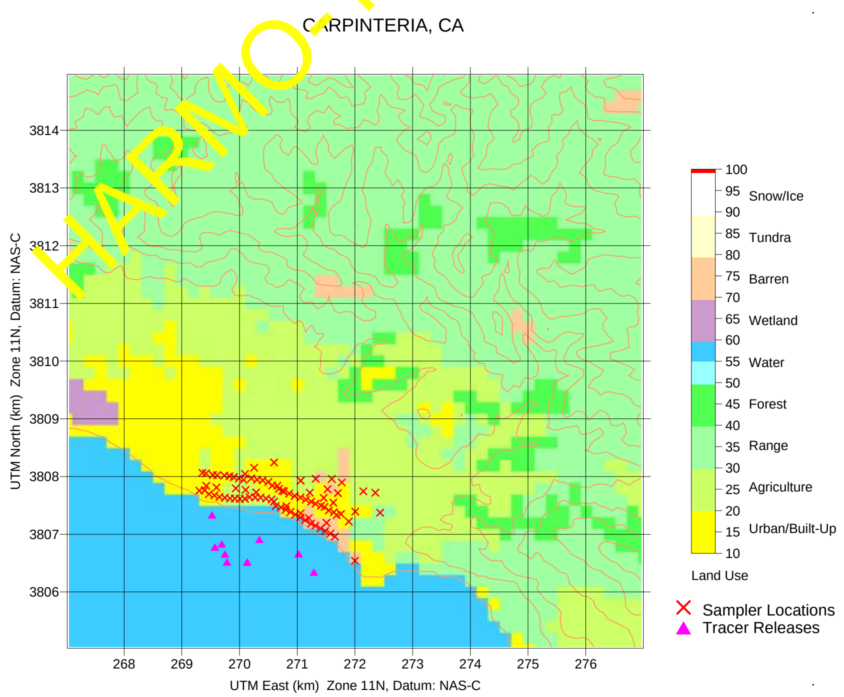
Summary and Conclusions

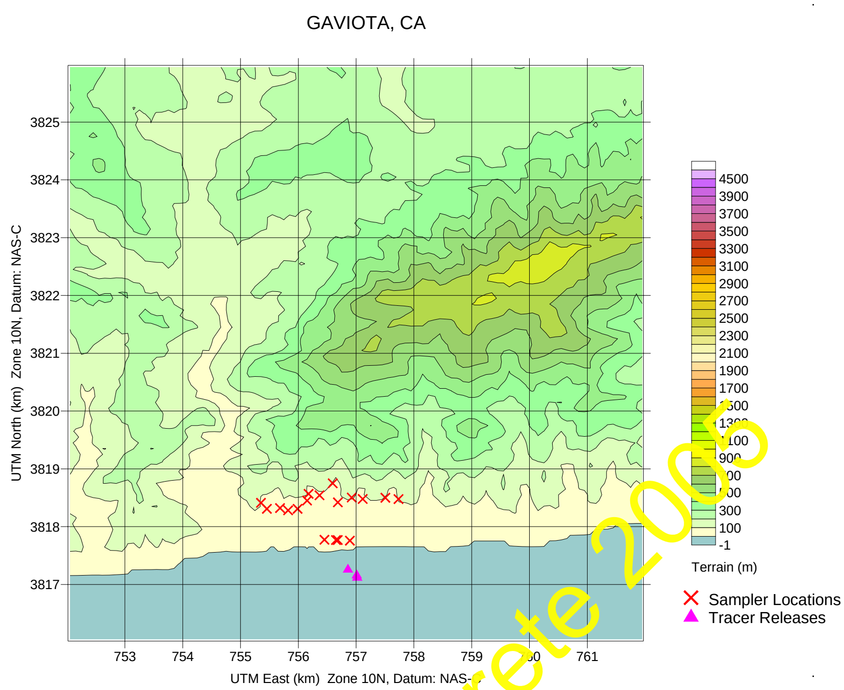
- The Batchvarova-Gryning (B-G) convective mixing height option in CALMET performs somewhat better than the Maul-Carson (M-C) option.
- Computed Lagrangian timescale approach for lateral dispersion leads to large overpredictions in CALPUFF. Existing Draxler approach performs better.

End

Evaluation Datasets

- OCD datasets (cont.)
  - Parallel evaluation to that done for OCD4, with emphasis on peak impact
  - CALMET/CALPUFF input data developed from OCD4 evaluation datasets
  - Transport direction inferred from peak observed impact
  - Dense line of model receptors along sampler lines
  - Performance assessment includes OCD5 results





Confidence Limits

– Bootstrap resampling technique applied to estimate 95% Confidence Limits

– MG and VG for peak modeled and observed χ/Q, paired in time

– Differences in MG and VG among models and model configurations

– Resampling blocks are chosen to preserve the representation of each site, and seasonality (e.g., each resampled set contains 17 entries for "Cameron Winter", which are randomly chosen with replacement from the 17 periods that comprise "Cameron Winter")

Blocking

– Ventura Fall	9	Periods
– Ventura Winter	8	Periods
– Pismo Beach Summer	16	Periods
– Pismo Beach Winter	15	Periods
– Cameron Summer	9	Periods
– Cameron Winter	17	Periods
– Carpinteria SF_6	18	Periods
– Carpinteria Freon	9	Periods
– Carpinteria Fumigation	9	Periods
– Gaviota	21	Periods
– Oresunde	9	Periods

Evaluation Statistics

- Model evaluation software package
- Measures

$$MG = \exp(\overline{\ln(Co/Cp)})$$

$$VG = \exp(\overline{(\ln(Co/Cp))^2})$$

$$R = \overline{(\ln Co - \overline{\ln Co})(\ln Cp - \overline{\ln Cp})} / (\sigma_{\ln Co}\sigma_{\ln Cp})$$

$$FAC2 = fraction \quad 0.5 \le (Co/Cp) \le 2$$

CALMET Grids

Vertical: 8 layers

- ZFACE(m) = 0., 20., 40., 60., 100., 200., 500., 1000., 3000.

Horizontal:

SITE	NX	NY	CELL SIZE (m)	Terrain Data (m)
Cameron	135	65	200	90
Carpinteria	100	100	100	30
Pismo Beach	100	130	200	90
Ventura	115	100	200	90
Gaviotta	100	100	100	30
Oresund	100	100	1000	900

CALMET Surface Met Data

(Cameron, Carpinteria, Pismo Beach, Ventura)

- Hourly meteorology derived from OCD applications
- 1 surface station, 1 upper-air station, 1 sea station
- Primary emphasis on overwater data (SEA.DAT)
- Wind direction from source to peak observed
- “Observed” overwater mixing height and dT/dz
- Measured RH and T(air)-T(sea)
- Measured wind speed near release
- Clouds from nearby observations

CALMET Met Data Aloft

(Cameron, Carpinteria, Pismo Beach, Ventura)

- Locate upper-air station away from study area
- Create 2 soundings/day (00Z and 12Z) using observation nearest 00Z
- Resolve overwater 2-layer structure (onshore flow)
- Observed dT/dz below mixing height, and default dT/dz = -.0045 deg/m above
- Wind direction constant
- Wind speed profile below mixing height from neutral or unstable power law (OCD stability class)
- Wind speed constant above mixing height

CALMET Runs

5 CALMET Runs each experiment

Site	Fluxes	Water Depth	Mixing Height
Ventura, Pismo, Carpinteria, Gaviota, Cameron	OCD COARE(wave 0) COARE(wave 0) COARE(wave 1) COARE(wave 2)	NA Deep Water Shallow Water NA NA	B-G / SEADAT B-G / SEADAT B-G / SEADAT B-G / SEADAT B-G / SEADAT
Oresund	OCD COARE(wave 0) COARE(wave 0) COARE(wave 1) COARE(wave 2)	NA Deep Water Shallow Water NA NA	B-G B-G B-G B-G B-G

CALPUFF Runs

4-16 CALPUFF Runs each experiment for each CALMET run

Site	**Turb (z-profile)**	**Iy**	**Fy Timescale**	**Terrain**
Ventura, Pismo, Cameron	CALPUFF AERMOD	Modeled Observed	Draxler Fy Variable	PPC
Carpinteria, Gaviota,	CALPUFF AERMOD	Modeled Observed	Draxler Fy Variable	PPC Strain
Oresund	CALPUFF AERMOD	Modeled	Draxler Fy Variable	PPC