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Technical Note

DESCRIPTION OF THE SST DATA ASSIMILATION SYSTEM USED IN THE NOAA COASTAL OCEAN FORECAST SYSTEM (COFS) FOR THE U.S. EAST COAST

Version 3.2*

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1. Introduction

The purpose of NOAA Coastal Ocean Forecast System (COFS) is to provide nowcasts and short-term forecasts of water temperature, salinity, water level, and currents for the East Coast of the United States. The development of COFS as well as other forecast systems for estuaries and the Great Lakes was begun due to the growing demand for surface and subsurface forecasts. This demand was recognized by the U.S. National Research Council, which recommended that the nation establish an "operational capability for nowcasting and forecasting oceanic velocity, temperature, and related fields to support coastal and offshore operations and management" (NRC, 1989).

COFS is a collaborative project between the National Weather Service (NWS), the National Ocean Service (NOS), and Princeton University. COFS has been run each day on the National Centers for Environmental Prediction (NCEP) Cray supercomputers since August 1993 to produce short-term simulations of the physical conditions of the coastal ocean off the U.S. East Coast (Aikman et al., 1994). Additional background information on COFS can be found in Aikman and Rao (1999), Breaker and Rao (1998), and Aikman et al. (1996). Specific information on data management, input and output files, and run scripts is described in Lobocki (1996).

A data assimilation cycle for COFS was developed and implemented semi-operationally on April 1, 1998. This version of COFS is referred to as COFS 3.2. The purpose of the cycle is to provide a three-dimensional nowcast of the coastal ocean physical structure. This nowcast provides the initial conditions for the daily COFS 24-h forecast cycle. The data assimilation cycle of COFS Version 3.2 assimilates both in-situ and remotely-sensed sea surface temperatures (SST). COFS 3.2 stopped running on September 27, 1999 when a fire destroyed the NCEP Cray C-90 (Cray3) supercomputer in Suitland, MD.

The COFS data assimilation system is based on three assimilation schemes, an optimal interpolation scheme (Derber and Rosati, 1989; Behringer, 1994; Behringer et al., 1998), a mixed-layer assimilation method (Chalikov et al., 1996), and Newtonian nudging. The optimal interpolation is used to determine a correction field for the temperatures of the model's top layer. The mixed-layer assimilation scheme is used to project the surface correction into the model's mixed-layer. Newtonian nudging is used to slowly apply a correction field to the model's mixed-layer.

This technical note documents the SST data assimilation system including a brief description of the coastal ocean model, the surface water temperature data, the method used to consolidate SST data from various observing platforms, the quality control procedures, and the data assimilation procedure. The last section contains a discussion of potential improvements for COFS.

2. Coastal Ocean Circulation Model

The basis of the COFS is a 3-D hydrodynamic ocean circulation model (Fig. 1) that has been developed jointly by Princeton University, NOS' Coast Survey Development Laboratory, and NCEP's Environmental Modeling Center, Ocean Modeling Branch. The model commonly referred to as the Princeton Ocean Model (POM) is based on the primitive equations, employs a free surface, and has a turbulent closure sub-model (Mellor and Yamada, 1982). The model explicitly predicts temperature, salinity, currents, free-surface water elevation, and turbulent quantities. POM uses the traditional hydrodynamic equations for conservation of mass, momentum, temperature, and salinity coupled by an equation of state. The primary simplifications are the hydrostatic assumption, the beta plane approximation, and the Boussinesq approximation with respect to density variation (Blumberg and Mellor, 1983). Detailed descriptions of the model equations and code can be found in Blumberg and Mellor (1983; 1987) and Mellor (1996).

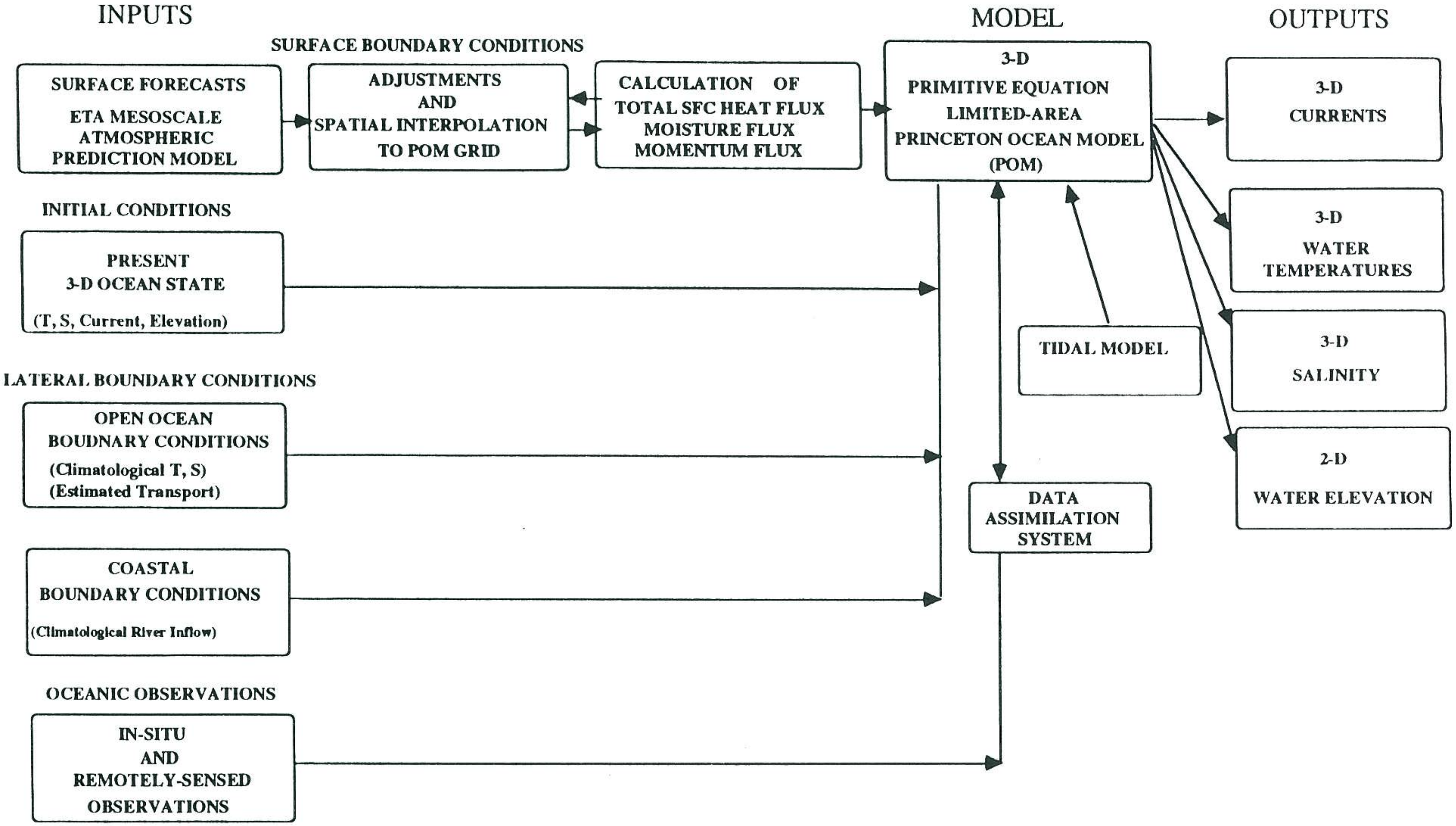

Figure 1. Flowchart depicting the inputs, outputs, and components of the NOAA Coastal Ocean Forecast System for the U. S. East Coast.

a) Grid Configuration

The COFS domain covers the region off the U.S. East Coast from approximately 30 to 47°N latitude and from the coast to 50°W longitude (Fig. 2). The coastal boundary corresponds to the 10 m isobath on the continental shelf. The version of POM used in COFS employs a bottom-following sigma coordinate system in the vertical and a curvilinear orthogonal grid in the horizontal. The spatial resolution of the model in the horizontal varies from approximately 20 km offshore to 10 km nearshore. A similar domain and horizontal resolution was used by Ezer et al. (1993) and Ezer and Mellor (1994) for experiments in data assimilation and POM. In the vertical, a 19-level sigma coordinate system is used with at least half the layers in the upper 100m. The 19 levels are: 0.0, -0.004, -0.0008, -0.0016, -0.0032, -0.0064, -0.0128, -0.0256, -0.0500, -0.1000, -0.200, -0.300, -0.4000, -0.5000, -0.6000, -0.7000, -0.8000, -0.9000, and -1.0000.

Model bathymetry is based on the U. S. Navy DBDB-5 (Digital Bathymetric Data Base on a 5 minute grid), modified over the continental shelf with the more accurate NOS bathymetry NOS-15 (15 second grid). The modifications were performed by Eugene Wei of NOS in the following manner. For a water cell of the COFS grid, the existing water depth based on DBDB-5 was replaced by the average of the NOS-15 data within a circle centered at the cell-center with a radius defined as the minimum of half of the cell size. The bathymetry refinements were conducted over the continental shelf and slope from the Florida Straits to about 44^{0}N. Erroneous high elevations over the outer shelf in the DBDB-5 bathymetry were corrected and the shelf break and continental slope were extended slightly offshore. The grid information for COFS is contained in the file *inhts.cfs*.

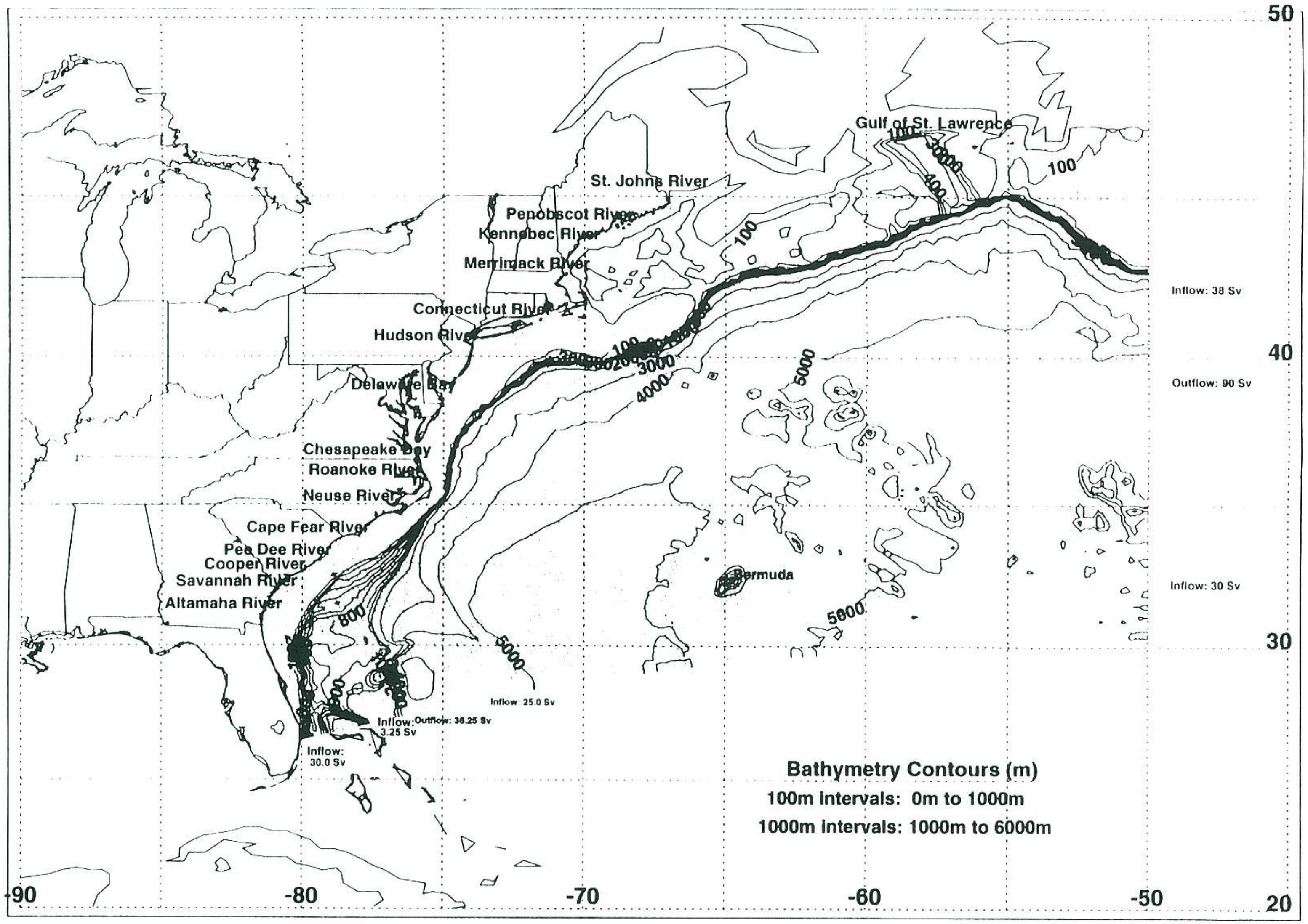

Figure 2. Location of “center” grid points of COFS, contours of model bathymetry, names and approximate locations of rivers for which outflow is specified, along with the amount of transport and where it is specified on the lateral open boundaries.

b) Lateral Boundary Conditions

Since there is presently no appropriate operational global or basin-scale forecast model covering the Atlantic Ocean Basin to provide open boundary conditions, POM is driven along its eastern and southern boundaries by the monthly climatological estimates of temperature and annual climatological estimates of salinity and transport. The temperature and salinity values are based on the U.S. Navy's Generalized Digital Environmental Model (GDEM) (Teague et al., 1990). The annual salinity boundary conditions (SBE and SBS) are contained in the file, *inhts.cfs* and was created by the POM group at Princeton University. The mean monthly temperature boundary conditions (TBE and TBS) are contained in the file *tbs_tbe.mon*. and was also created by the POM group. No procedures were performed on the interpolated GDEM climatology to check for vertical static instability or non-smoothness of the temperature and salinity fields.

The transport of water in and out of the domain is specified on open boundaries as depicted in Fig. 2. On the southern boundary, an inflow of 58.25 Sverdrups (Sv) and outflow of 36.25 Sv are prescribed and distributed horizontally based in part on the measurements from the Subtropical Atlantic Climate Studies (STACS) program (Leaman et al., 1987). One Sverdrups is equal to 106 $m^{-3}s^{-1}$. On the eastern boundary, a total of 90 Sv are allowed to exit the domain between 37° to 40°N, while a total inflow of 38 Sv enters north of the Gulf Stream, along the continental slope, and 30 Sv enters south of Gulf Stream. The northern and southern inflows on the eastern boundary, which are based on diagnostic calculations and observations (Richardson, 1985), represent the northern recirculation gyre and subtropical gyre, respectively. The internal and external velocities are set in the subroutine VABFIX.

Monthly estimates of fresh water input into POM are prescribed for 15 major rivers or estuaries and the Gulf of St. Lawrence (Fig. 2) based on the monthly climatology of Blumberg and Grehl (1987) and Koutitonsky and Bugden (1991), respectively.

According to Blumberg and Grehl (1987), the 15 rivers/estuaries account for almost 90% of the total fresh water discharge into the eastern continental shelf region.

The fresh water inflows are specified using the DATA statements in subroutine RUNOFF. This subroutine is called at each internal time step following the calculation of the salinity at the forward time step in subroutine ADVT. The particular month used for any COFS run is based on MON, the month of the year. The MON is calculated from MM which is passed from the main program. There appears to be no temporal interpolation between months.

For all estuaries, the mean runoff for any month is linearly interpolated in the vertical. This causes the maximum effect on salinity at the model's top sigma layer and zero effect at the bottom layer. In the case of the Gulf of St. Lawrence, the runoff is restricted to the top 100m. The estuarine and Gulf salinities are assumed to be zero, but is not directly specified in the subroutine. The overall approach to modifying the salinity at an estuary or the Gulf is based on the following. Fresh water mixes with saline water instantly to produce less saline water at one grid cell so that only runoff and time step are needed explicitly (Chen, personal communication, 1997). For all estuaries, the salinity at the estuary mouth grid point is calculated by

```
S(I,J,K)=S(I,J,K)-S(I,J,K)*ROFF(N,MON)*(2.+Z(K)+Z(K+1))*DTI2/(ART(I,J)*D(I,J))
```

where S is the salinity calculated previously in subroutine ADVT, ROFF is the monthly runoff value for a particular estuary (N) and month (MON), Z is the non-dimensional depths of the sigma level, DTI2 is twice the internal model time step, ART is the area of the grid box centered at the model's depth grid point, and D is the instantaneous depth. The quantity (2.+Z(K)+Z(K+1)) provides the linear decrease with depth.

For the Gulf of St. Lawrence, the salinity is calculated in the following manner:

```
DEPTH=D(I,j)*ZZ(K)
FACTOR=2.0+DEPTH*2.0/100.0
IF(DEPTH.LT.-100.0)FACTOR=0.0
S(I,J,K)=S(I,J,K)-S(I,J,K)*ROFF(N,MON)*FACTOR*DTI2/(ART(I,J)*100.0
```

where ZZ is the nondimensional depth of a sigma layer. Additional information on the effect of fresh water flow on COFS salinity and current fields can be found in Breaker et al. (1999).

c) Surface Boundary Conditions

The model is driven at its upper boundary by forecasts of heat, moisture and momentum fluxes from the 0000 UTC forecast cycle of NCEP's Eta atmospheric forecast model (Black, 1994; Rogers et al., 1998; Rogers et al., 1999). Eta fluxes and meteorological variables at 3 hourly intervals are interpolated to the COFS grid using the Fortran program, *intp31.f* and stored in the file, *eta.flx.* COFS has the ability to use Eta forecasts from previous cycles if there are missing forecasts in the 0000 UTC cycle.

Sensible and latent heat fluxes for COFS are not taken directly from Eta's fluxes, but are instead calculated from the Eta model's surface meteorological forecasts (i.e. air temperature, specific humidity, u and v surface [10 m AGL] wind components) and in part on POM's SST and top model layer currents. The calculations are done in the subroutines SURF_F and FLUX of the Fortran programs, *pomcfs32n.f* and *pomcfs32f.f.* The Eta model's downward short wave and upward long wave radiation fluxes are adjusted to account for known biases in the Eta model. Short wave radiation values are multiplied by 0.8 (zetaS) and downward long wave radiation values are multiplied by 1.054 (zetaL) in the Fortran program *intp31.f.*

COFS has been using the Eta-32 forecasts since June 4, 1998 when Eta-29 was discontinued. Eta-32 has a horizontal resolution of 32 km with 45 layers in the vertical. The domain of the Eta-32 model is depicted in Fig. 3. For its specification of SSTs, the

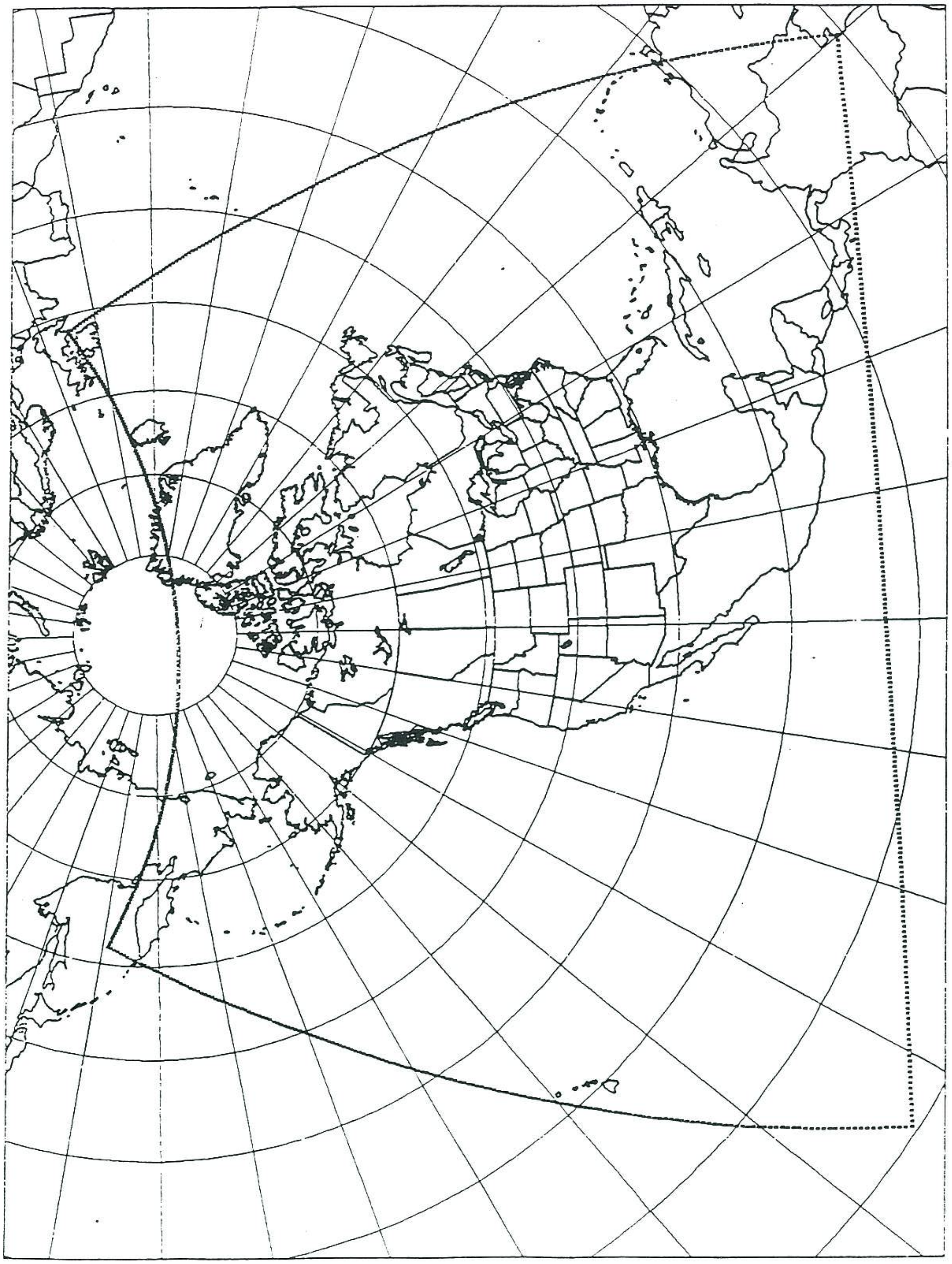

Figure 3. The grid domain of NCEP's 32 km version of the Eta atmospheric prediction model.

Eta-32 model uses NOAA's National Environmental Satellite, Data and Information Service (NESDIS) 50-km resolution Multi-Channel Sea Surface Temperature (MCSST) Analysis that is updated approximately twice a week. Initial conditions for the Eta forecast cycle are provided by the Eta Data Assimilation System (EDAS).

The COFS short-term archive of Eta-32 forecasts (GRIB format) out to 36 hours can be found in the files *YYMMDD00sf32.grb* in the directory: */ombptmp/cfspom/archives/eta/32km/YYMM*. Presently, a parallel run of the COFS nowcast/data assimilation cycle is being conducted which uses 3 hourly analyzed fields from EDAS as a replacement to the Eta forecast fields. If successful, the COFS nowcast/data assimilation cycle will use analyzed fields from EDAS and the COFS forecast cycle will use forecast fields from the Eta-32 model.

d) Tidal Forcing

Tidal forcing was implemented in COFS Version 3.1 on November 15, 1996. It includes tidal boundary forcing on the eastern and southern lateral open boundaries of COFS via tidal barotropic currents and astronomical tidal forcing within the COFS domain via tidal elevations. Astronomical tidal forcing is also referred to as body or equilibrium tidal forcing and is due to the gravitational attraction between ocean particles and the moon and sun. The tidal forcing algorithms were developed by the POM group at Princeton University (Chen and Mellor, 1999).

The tidal boundary forcing via tidal currents on the open boundaries is accomplished in the following manner. A 2-D (depth-averaged), linearlized version of the POM with lateral boundary conditions and astronomical tidal forcing based on Schwiderski global tidal work along with corrections for effects of "earth tide" and "ocean loading tide" (Schwiderski, 1980) was run for two-years. Both the boundary and astronomical tidal forcing included three semi-diurnal constituents: principal lunar (M2), principal solar (S2), and lunar elliptic (i.e. changing distance between earth and moon) (N2), and three diurnal constituents: luni-solar (K1), principal lunar (O1), and principal solar (P1). An optimization scheme was then used to obtain a set of optimal "tidal pulse modes" coefficients for amplitude and phase for both elevation and velocity by minimizing the summed error between the model's estimates and the observed tides at water level gage stations, plus the difference between the model open boundary tides and the model first guess boundary tides (Chen and Mellor, 1999). These coefficients for six constituents along the eastern and southern boundaries are stored in the binary file *tide6.bdr* and are read by subroutine TIDE_SETUP. The tidal elevation amplitudes and phases are stored in the variables EAMPE and EAMPS and EPHAE and EPHAS, respectively. The tidal u-velocity amplitudes and phases are stored in the variables UAMPE and UAMPS, and UPHAE and UPHAS, respectively. A similar set of variables was assigned for the v-velocities. In addition, ad hoc fixes are applied to the amplitudes (AMP_CO=0.45) and phases (PHA_CO=-100.0) of the tidal elevation and tidal velocities for the three-diurnal constituents on both open boundaries.

The astronomical or equilibrium tidal forcing within the COFS domain in terms of amplitudes and frequencies for the six constituents are specified from Schewiderski global tidal model and assigned to the variables AMP and OME in the DATA statements of subroutine TIDE_SETUP. These variables are used in the subroutine TIDE_BODY to calculate the equilibrium tide which is stored in the variable EEQ.

In the subroutine BCOND, the tidal currents, UTIDE and VTIDE are calculated based on the tidal velocity amplitude and phase coefficients for the eastern and southern boundaries, respectively. UTIDE and VTIDE are then used as one set of the external velocity boundary conditions. In addition, the tidal elevation ETIDE is calculated for both open boundaries and is based on the tidal elevation amplitudes (EAMPE or EAMPS) and phases (EPHAE or EPHAS). ETIDE is used along with the other elevation boundary condition, the non-tidal mean boundary elevation (i.e. ELE and ELS) to calculate total elevation. The values of ELE and ELS were obtained from a two-year run of the non-tidal run of POM and stored in the file, *els_ele_.2yr.* (ELE and ELS are sometimes referred to as long-term "error" corrections.) The resultant elevation is then converted to a velocity by multiplying it by the SQRT(GRAV/H), where GRAV is gravity at sea level and H is bottom depth.

Finally, in subroutines ADVU and ADVV, the equilibrium tide EEQ together with the inverted barometric pressure, are used in the computation of the pressure gradient term.

e) Parameterizations

The parameterization of turbulent mixing is accomplished using a Level 2.5 turbulence closure scheme of Mellor and Yamada (1982) as modified by Galperin (1988). The closure scheme is used to obtain expressions for the vertical eddy diffusivities in the model conservation equations for temperature, momentum, and the turbulent quantities. The turbulent Prandtl number (TPRNU) is set to 1.0.

The horizontal diffusion terms representing motions induced by small-scale processes not resolved by the model are parameterized in analogy to molecular diffusion. However, horizontal viscosity and diffusivity terms are required to damp small-scale computational noise Blumberg and Mellor (1987). These terms are specified according to the formulation of Smagorinsky (1963) which takes into account the vertical variability in the horizontal viscosity and diffusivity. The non-dimensional empirical constant (HORCON) used in the Smagorinsky formulation is set to 0.1.

f) Numerical Methods

The model equations together with their boundary conditions are solved using a mode splitting technique, spatial and temporal finite difference techniques and a staggered horizontal grid. The model splits or separates the model equations into two "modes" called the internal (baroclinic) and external (barotropic) modes. The time steps of the internal and external modes are 720 and 16 seconds, respectively.

An Arakawa-C staggered grid structure (Arakawa and Lamb, 1977) is used in the model. A centered finite difference method is used to solve the model equations. In this method the difference is computed from grid points symmetrical about the point where the difference is required (Mesinger et al., 1990).

The finite difference equations are advanced forward in time using a "leapfrog" scheme, a three-level time differencing method. The Asselin-Roberts time filter (Roberts, 1966; Arakawa, 1972) is applied at the end of each internal model calculation to remove "time splitting" introduced by the leapfrog scheme. The constant used in the time filter (SMOTH) is set to 0.10.

g) Daily Execution Procedure

The COFS 3.2 data assimilation cycle is launched each day by the shell script *archearly.sh*, found in directory: */ombptmp/cfspom/archives/software*. The script submits the script: *launcher.cofs32n.qsub,* as a batch job to NCEP's Cray C-90, commonly referred to as Cray3. This script executes the C program *run32n.c:* which performs a variety of tasks including:

1) executing *intp32.f* to interpolate ETA-32 surface variables to the COFS grid,

2) selection of SST observation files for the given day,

3) creation and submittal of shell script *cofs32n.qsub* to run POM via the execution of *pomcfs32n.x*, and

4) creation of shell script *www-cofs32n.qsub* to transfer POM output to an NCEP workstation and to activate IDL-related scripts on an SGI workstation to display COFS output on the NCEP/EMC Ocean Modeling Branch's WWW site: http://polar.wwb.noaa.gov.

More detailed information on COFS execution scripts and output files can be found in Lobocki (1996).

3. Types of SST Data

SST observations are obtained from both in-situ and remote-sensing platforms. The in-situ platforms include drifting and fixed buoys, Coastal-Marine Automated Network (C-MAN) stations, and ships participating in the Voluntary Observing Program. Remotely-sensed observations include MCSST retrievals from the Advanced Very High Resolution Radiometer (AVHRR) on board the NOAA-14 and NOAA-15 polar-orbiting satellites. An example of the number and location of SST observations for a 48-h period is depicted in Fig. 4. On this particular two-day period, there was excellent data coverage in the COFS domain.

a) In-Situ SST Observations

1) Drifting Buoys

Drifting buoys consist of NOAA's Global Lagrangian Drifters (GLD) and International Ice Patrol Buoys. The GLDs measure water temperature only (Bushnell, 1996, personal communication). The water temperature sensor is located a few inches below the water surface. Most GLDs are equipped with *Holey-Sock* drogues and a drogue sensor to signal drogue loss. The movement of GLDs with drogues are largely dependent upon ocean currents.

The data from the drifters are transmitted by UHF communications via NOAA polar-orbiting satellites to NESDIS ground receiving stations and then relayed to the U.S. Global Processing Center (GPC) in Landover, MD, for processing and dissemination to the National Weather Service Telecommunications Gateway (NWSTG). Data from drifting buoys are transmitted in WMO FM18-IX BUOY code.

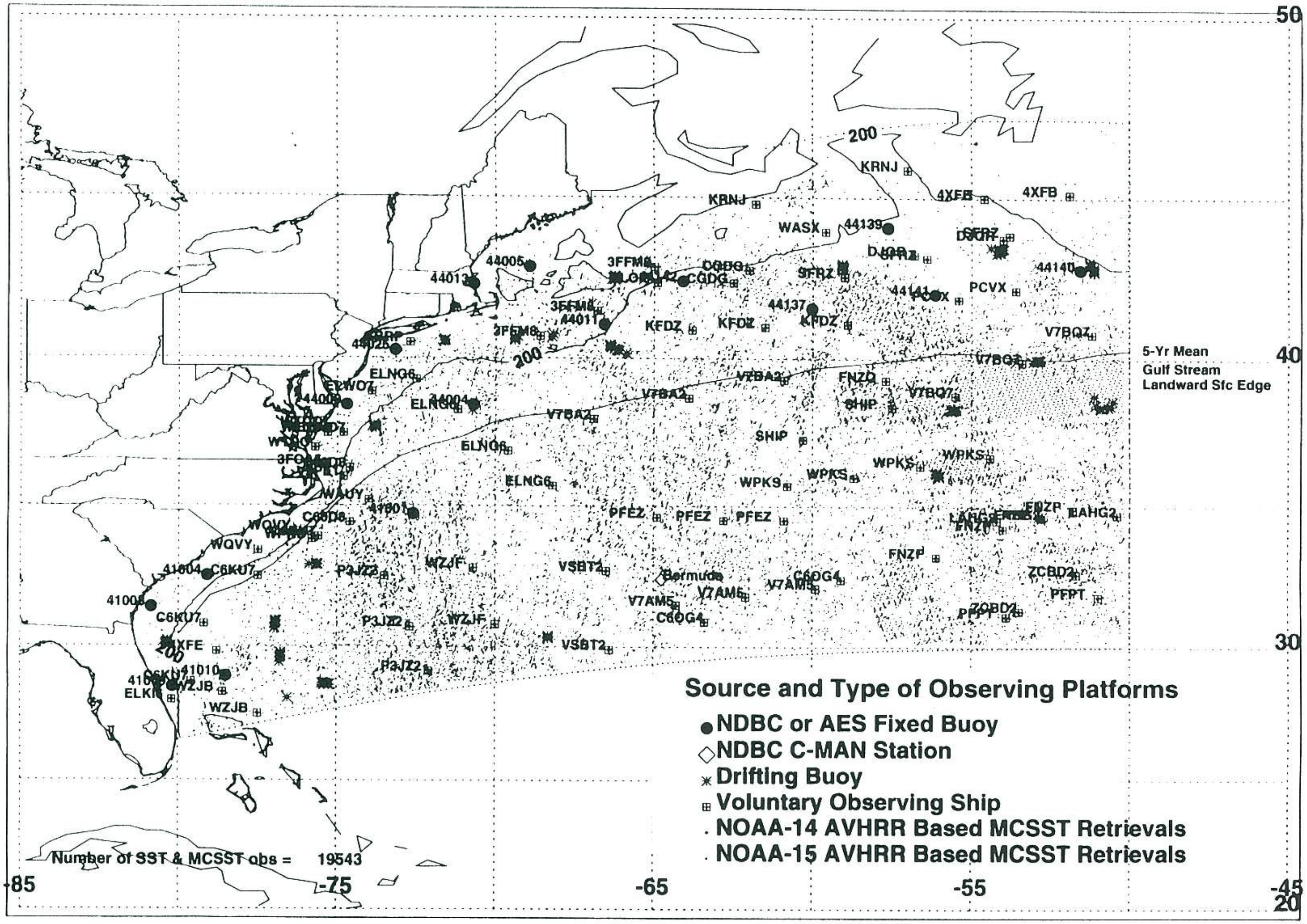

Figure 4. Example of the location and different types of SST and MCSST observations available in the COFS domain during a 48-h period. The IDs for in-situ platforms (except drifting buoys) are given. Also shown are the 200m isobath and a 5-year mean Gulf Stream landward surface edge.

Information about the GLDs is available at NOAA's Global Drifter Center located at AOML in Miami, FL. The information includes records of individual drifters, such as dates of deployment, sensor failure and removal from GTS distribution, total transmission failure, *etc*...This record is updated monthly by GDC's Data Assembly Center (DAC). The GDC maintains a WWW site:

http://www.aoml.noaa.gov/phod/dac/gdc.html.

Observations from drifting buoys are archived in the World Meteorological Organization (WMO) **B**inary **U**niversal **F**orm for **R**epresenting Meteorological Data (BUFR) format at NCEP. The observations are stored on one of NCEP's Cray J-90 supercomputers, commonly referred to as Cray4, in file *xx002* under the directory:

/dcom/us007003/YYYYMMDD/b001, where *YYYYMMDD* represents year, month, and day.

2) NDBC and AES Fixed Buoys

Moored buoys routinely acquire and transmit hourly data. The data consist of sea-level pressure, wind speed and direction, air temperature, sea-surface water temperature, significant wave height and period, and wave spectral data. The NDBC fixed buoy observations are checked at the NWSTG using a NDBC validation method. The method includes a range check and a standard-deviation-based, time continuity check (GIlhousen, 1988; Gilhousen, 1998). Typical limits for the water temperature check are –2 to 40.0°C. The standard deviation used for the time-continuity check of water temperature is 8.6°C, except it is12.1°C for East Coast stations in the vicinity of the Gulf Stream (Gilhousen, 1998). The status and capability of the U.S. buoys can be obtained from the National Data Buoy Center (NDBC) WWW site,

http://seaboard.ndbc.noaa.gov.

Observations from fixed buoys are archived in BUFR format at NCEP. The observations are stored on Cray4 in file *xx003* under the directory:

/dcom/us007003/YYYYMMDD/b001.

3) NDBC Coastal-Marine Automated Station Network

C-MAN stations routinely acquire and transmit data every hour. The data consist of sea-level pressure, wind speed, wind direction, and air temperature. Some C-MAN stations report sea-surface water temperature, water level, significant wave height and period, and wave spectral data. C-MAN observations are checked at the NWSTG using the same NDBC validation method as for the NDBC fixed buoys.

The status and capability of the U.S. C-MAN stations can be obtained from the NDBC WWW site, *http://seaboard.ndbc.noaa.gov*. In addition, a monthly status summary is received at NCEP's Environmental Modeling Center/Ocean Modeling Branch via U.S. Mail. Additional information about C-MAN stations can be found in *The Coastal Marine Automated Network (C-MAN) NWS User Guide*.

Observations from C-MAN stations are available at NCEP in BUFR format. The observations are stored on Cray4 in file *xx004* in the directory:

/dcom/us007003/YYYYMMDD/b001.

4) Voluntary Observing Ships

SST observations are measured by ships participating in the Voluntary Observing Ships (VOS) program by a variety of methods: bucket, engine intake, or hull contact sensors at depths usually between 3 and 9 m (Kent et al., 1993). A informal survey of NOAA research ships in 1998 indicated a similar variety of methods and measurement depths.

The ship name and agent name associated with each ship can be found in the NWS VOS Program Call Sign List publication. However, this publication does not provide the depth of SST sensors or method of measurement. This publication is available from the VOS Program Leader in the NWS Marine and Applied Sciences Branch in Silver Spring, MD.

Observations from ships participating in the VOS program are available at NCEP in BUFR format. The observations are stored on Cray4 in file *xx001* under the directory:

/dcom/us007003/YYYYMMDD/b001.

5) METAR Stations

There are many aviation routine weather reporting surface stations (METAR) along the East Coast. Presently, these stations do not include SST measurements. Additional information on METAR sites and the reporting format can be found at http://tgsv5.nws.noaa.gov/oso/oso1/metar.htm.

Observations from METAR sites are available on Cray4 in the file *xx007* in the directory: */dcom/us007003/YYYYMMDD/b000.*

6) NOS Water Level Stations

SST observations are measured at water level and meteorological observing stations operated by NOS' Center for Oceanographic Products and Services. The gages report via GOES at approximately 3 hour intervals, with plans for hourly transmission in the near future. The observations are transferred from NOS to NWS/OSO in the WMO format, **C**haracter form for the **R**epresentation and **EX**change of data (CREX) (NOS, 1999) and the NWS **S**tandard **H**ydrometeorological **E**xchange **F**ormat (SHEF) (NWS, 1998). Presently, NCEP does not have a decoder to read CREX bulletins. Additional information on the NOS observing network can be found at http://www.co-ops.nos.noaa.gov/data_res.html.

It is anticipated that NOS will supply NCEP with a decoder during 1999. These observations are not available to COFS for assimilation at the present time.

7) USCG Stations

SST observations are measured at many U.S. Coast Guard (USCG) stations and by USCG personnel on local ship patrol. These observations are transmitted by NWS/OSO in plain text messages. The format of these messages varies by USCG region. These observations are presently not available to COFS for assimilation.

b) MCSST Retrievals

The NESDIS MCSST retrievals are derived from the AVHRR sensor onboard the NOAA-14 and NOAA-15 polar-orbiting satellites. These include both nighttime and daytime retrievals. A description of the equations used to derive SST retrievals from the AVHRR sensor on board the NOAA-14 satellite is given in Walton et al. (1998).

Each retrieval represents an approximate 8 km x 8 km or 64 sq. km box (Gockel, 1996, personal communication). The retrieval is based on an average of 4 AVHRR Global Area Coverage (GAC spots) arranged as a 2 x 2 “unit array”. Each GAC spot in the unit array is an approximate 4 km x 4 km square of 1km horizontal resolution AVHRR data. The averaging from 1 km to 4 km resolution is done on board the spacecraft. Detailed descriptions of the processing can be found in the *NOAA Polar Orbiter Data User's Guide* available on-line at http://www2.ncdc.noaa.gov/POD.

The MCSST retrievals are quality controlled in the following manner. First, there is a climatological test in the orbital processing stage that eliminates any retrieval which is greater than 10°C from climatology. In addition, a range check is done to eliminate any retrievals which are not in the range between –2 and 35°C (Sapper, 1999, personal communication).

NESDIS MCSST retrievals are archived for 7 days at NCEP. The retrievals are stored in BUFR format and located on Cray4 under directory:

/dcom/us007003/YYYYMMDD/b012.

The file name convention is *xx011*. These files contain all MCSST retrievals for a given "Greenwich day" (0000 UTC-2359 UTC). The file is updated six times a day. In addition, a daily BUFR file of MCSST retrievals based on U.S. Navy data processing procedures are available at NCEP in the same directory. The file containing the Navy retrievals is *xx010*.

4. Creation of Unified Surface Marine In-Situ Observation File for the COFS Region

Oceanographic and meteorological observations from the overwater and near-shore observing platforms listed in the previous section are decoded from the BUFR format and combined into a daily surface marine observation file (Fig. 5). The daily file is created by the shell script, *create-mobs-file.sh*, located in the directory: *ombptmp/cfspom/archives/software/sfcmobs*.

Only observations within the COFS region and Gulf of Mexico (25°–49°N latitude and 45° – 100°W longitude) are saved in the file. The area was expanded to cover the Gulf in anticipation of the future expansion of the COFS domain. The observations are stored in ASCII data format in a field format created specifically for the COFS project. The files are stored in the Cray3 directory:

/ombptmp/cfspom/archives/sfcmobs_data/YYYYMM.

Each observation contains the variables listed in Table 1. The identification codes used to indicate the type of observing platform are given in Table 2.

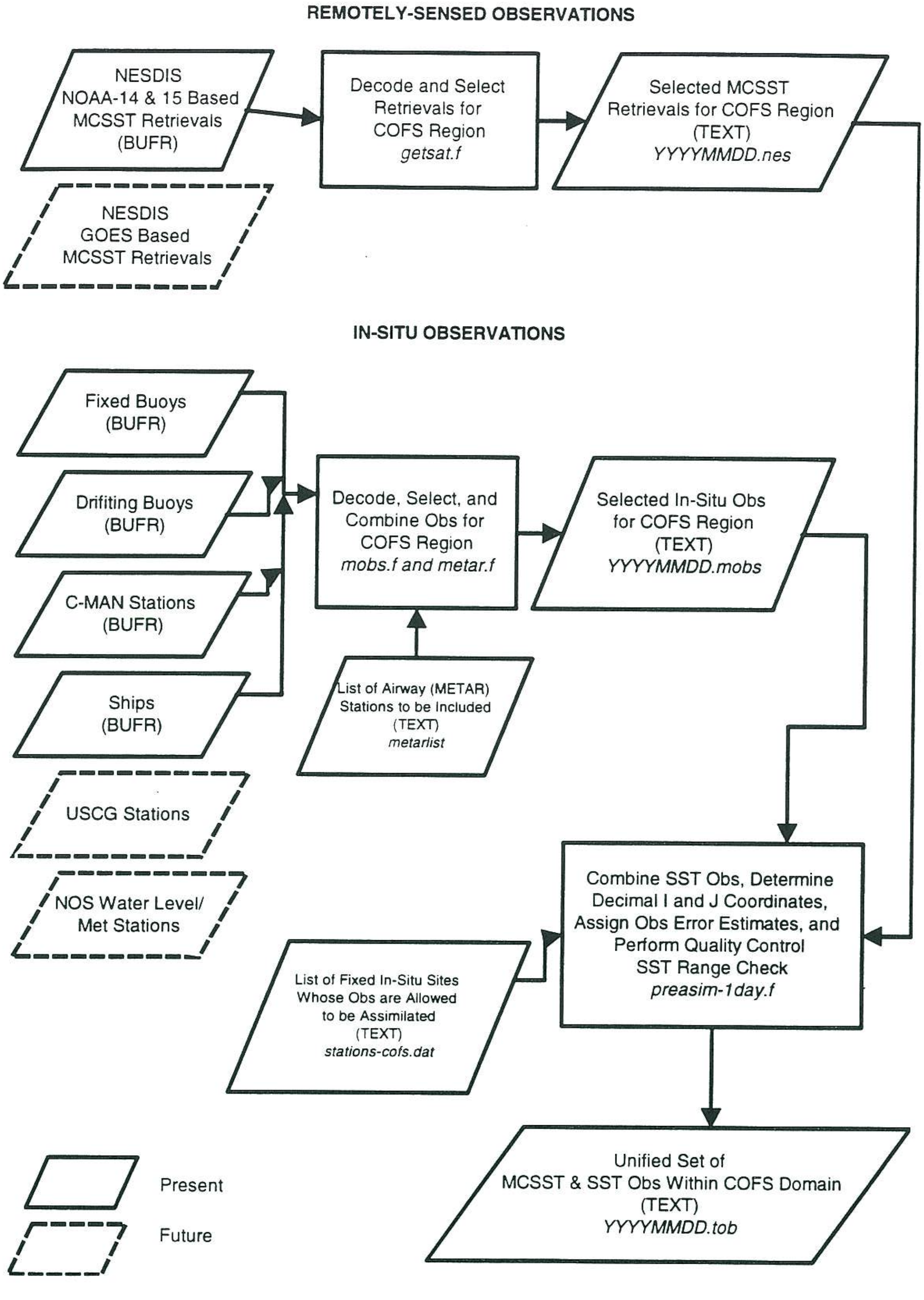

Figure 5. Flowchart depicting the data and steps used in the creation of a unified surface marine observation file for the COFS region.

Table 1. List of variables contained in the COFS surface marine observation file and their units.

Variable	Abbreviation	Units
Year (2 digit)	iyr	
month	mnth	
day	iday	
hour	ihrn	
minute	minu	
Observing platform ID	id	
Station type (COFS classification)	irpt	
Present weather (500 codes)	prewet	
Total cloud cover	cld	%
Visibility (horizontal)	visb	m
Mean sea level pressure	pmsl	mb
Air temperature	airt	deg C
Dew point temperature	dpd	deg C
Wind direction	wdir	degrees
Wind speed	wspd	m/s
Wind speed gust	wdgst	m/s
Wind speed estimated at 10m AGL	w10m	m/s
Observed sea surface temperature	sst	deg C
Quality controlled SST	qcsst	deg C
Height of waves	howw	m
Period of waves	poww	m
Observing site latitude	clat	degrees
Observing site longitude	clon	degrees
Height of wind waves	howv	m
Period of wind waves	powv	m

Notes: howw and poww are from wave instrumentation. howv and powv are usually visual observations from ships.

Table 2. Observing Platform Identification Codes used by COFS.

Code	Observing Platform
1	Ship
2	Drifting Buoy
3	Fixed Buoy
4	C-MAN Station
5	ASOS,AWOS, or manual aviation reporting station
151	NOAA-14 AVHRR – Daytime operational
152	NOAA-14 AVHRR – Nightime operational
159	NOAA-14 AVHRR – Daytime operational (relaxed cloud mask)
171	NOAA-15 AVHRR – Daytime operational
173	NOAA-15 AVHRR – Nightime operational
179	NOAA-15 AVHRR – Daytime operational (relaxed cloud mask)

If the platform does not report this variable, or, if it is missing for the given hour, then a –99.9 flag is placed in the field. The observation record was written using the Fortran formatted write statement:

```
write(11,65)iyr,mnth,iday,ihrn,minu,shipid,irpt,prwet,cld,visb,pms1,airt,dpd,wdir,wspd,w
dgst,w10m,sst,qcsst,howw,poww,clat,clon,howv,powv
format(1x,5i2,1x,a8,3i4,1x,2f8.1,2f7.1,1x,i3,7f7.1,1x,2f8.2,2f7.2)
```

The files are named using the convention: *YYYYMMDD.mobs*. Daily files have been created since August 13, 1996. The files have been permanently archived on CD-ROMs. In the future, surface marine observations from additional stations such as the NOS water level/meteorological observing stations will be added to the file.

5. Creation of the MCSST Retrieval File for COFS Region

A subset of the retrievals from the NESDIS MCSST file is extracted daily for the COFS domain (Fig. 5). This is accomplished by the shell script, *create-nes-file.sh* and the Fortran program *getsat.f* in Cray3 directory:

/ombptmp/cfspom/archives/software/retrvls.

The Fortran program uses the BUFR decoder program *bufrlib* in Cray3 directory */nwprod/bufrlib*. The script is submitted for execution at 0030 UTC each day. A log file containing information on the execution can be found in */ptmp1/cfspom/retrvls*. The ASCII file of retrievals created by *getsat.f* is archived in directory:

/ombptmp/cfspom/archives/retrvls/YYYYMM.

The file name convention is *YYMMDD.nes*. These files have been created since 1996.

6. Preparation of SST Data for the Data Assimilation System

The in-situ SST observations and MCSST retrievals within the COFS domain for a day are selected and combined into one ASCII file (Fig. 5). Observations from selected fixed buoy and C-MAN stations are withheld for use in verification. The buoys and stations were selected to evaluate COFS SST predictions near the coast, offshore, north and south of the Gulf Stream, and near an open boundary. A list of the stations that were not withheld is contained in the file *stations-cofs.dat*. The location of the sites are depicted in Fig. 6.

As the SST observations and retrievals are combined, the location of the retrievals and in-situ SST observations in model grid coordinates, *i.e.* decimal I and J, are calculated and added to the data record. This is accomplished by the Fortran program *preasim-1day.f*. The program is executed by the shell script *create-tob-file.sh* located in the directory:

/ombptmp/cfspom/CFS3.2n/pre.

Each data record in the daily SST file contains the time, date, latitude, and longitude coordinates, the corresponding model decimal I and J grid coordinates, sensor ID, observation type, water temperature, and the estimated reciprocal of the error variance. The identification codes used to indicate the type of observing platform are given in Table 2. The estimates of the measurement errors and variances for the in-situ and remotely-sensed observations are given in Table 3. The daily files of retrievals are stored in the directory:

/ombptmp/cfspom/CFS3.2n/oceanobs/tem/YYYYMM

using the filename convention *YYYYMMDD.tob*. The files have been permanently archived at NODC since 1998.

A range check is performed on all SST data. The SST data must be between 1° and 33°C. If not, the data are not included in the file of combined observations and retrievals. Additional quality control procedures, such as checks for geographic positional errors, are planned for COFS.

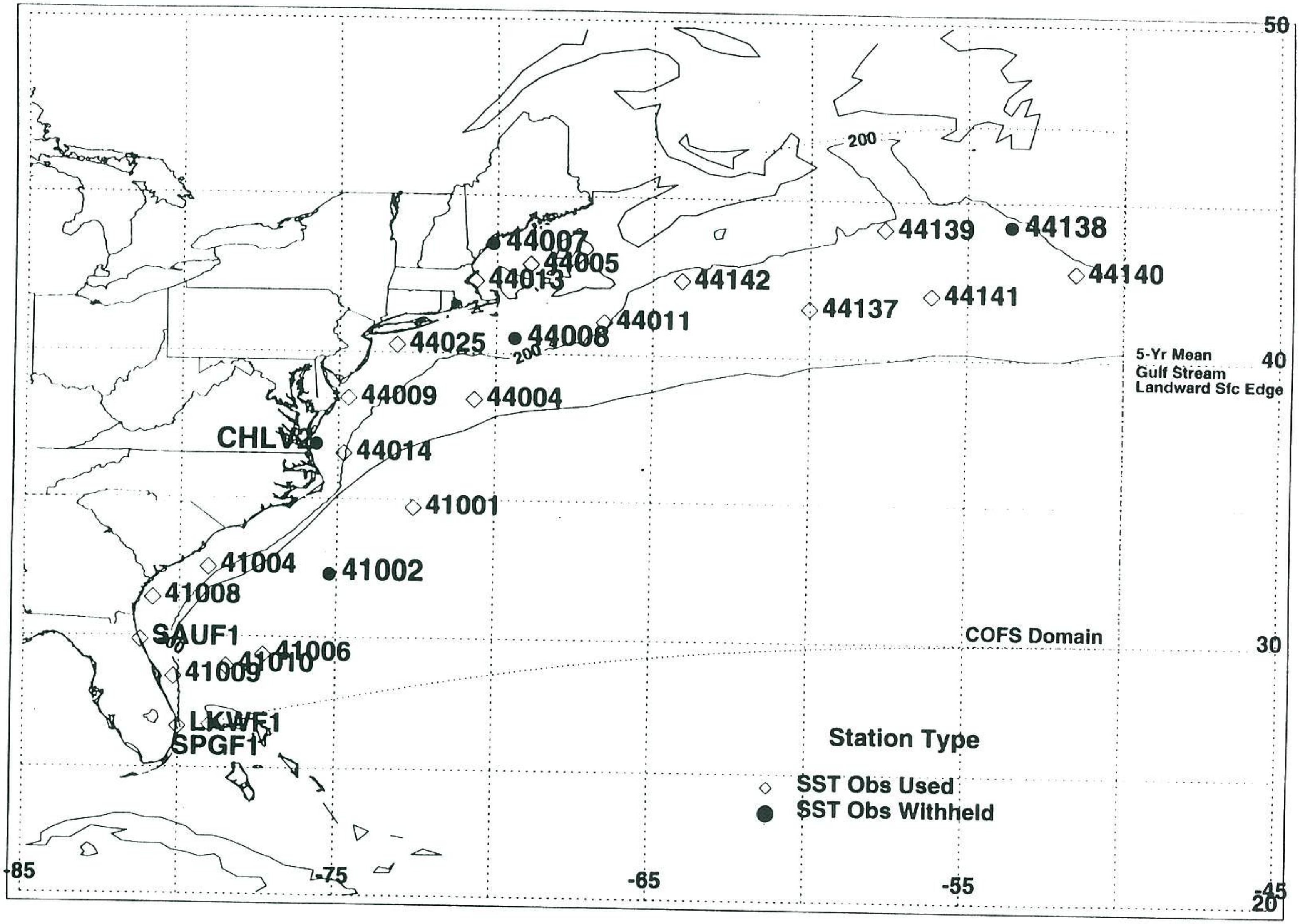

Figure 6. Locations of fixed platforms in the COFS domain whose SST observations were used or withheld from data assimilation. The 200m isobath and a 5-year mean Gulf Stream landward surface edge are also depicted.

Table 3. Measurement errors assigned to different types of observations used in COFS and other ocean data assimilation systems.

Ob Type	Measurement Error (°C)	Ref.	Error Variance (°C^2)	Recip. of Error Variance (°C^2)$^{-1}$	Measurement Error (°C)		
					Ji et al (1995)	Behringer (1994)	Renolds and Smith (1994)
MCSST Retrievals							
Day OP	0.31	Pichel et al (1995)	0.096	10.4	0.7	0.4	0.5
Day OP (warm spot)	0.40	none	0.160	6.3	Not known if this type of retrieval is being used in SST analysis		
Night OP	0.27	Pichel et. al (1995)	0.073^2	13.7	0.4	0.4	0.3
In-Situ							
Fixed Buoy	0.13	Gilhousen (1987)	0.017	58.8	NU	NU	NU
Drift Buoys	0.13	None	0.017°	58.8	0.1	NU	0.5
C-MAN	0.13	None	0.017	58.8	NU	NU	NU
Ships	1.0	None	1.000°	1.0	1.0	1.0	1-1.5

NU – Not used in assimilation
OP – Operational

Note: Presently, the Reynolds' analysis is being used as data in the Climate Modeling Branch's assimilation systems for their Atlantic and Pacific Ocean Models.

7. SST Data Assimilation System

The COFS SST data assimilation system is based on three assimilation schemes. In the first scheme, observed temperatures are assimilated into the model's top layer following the method of Derber and Rosati (1989) and Behringer (1994; 1998). In the second scheme, the correction field for the top model layer is projected downward into the mixed layer following the method of Chalikov et al. (1996). A similar extrapolation method was used by Forbes (1995) in the ocean data assimilation system of the United Kingdom Meteorological Office Forecasting Ocean Atmosphere Model (FOAM) for the Atlantic Ocean. Finally, a nudging procedure is used to slowly apply a three-dimensional correction field into the model's mixed-layer. A flowchart depicting COFS SST assimilation system is given in Fig. 7.

a) Derber/Behringer Assimilation Scheme

Using the terminology of Daley (1991), the overall approach of the Derber/Behringer method is the following. The model simulated SSTs, also referred to as *first-guess* or *background estimates,* are obtained at SST observation sites by bilinear interpolation. This interpolation of the background estimate to the observation site is referred to as *forward interpolation.* Background estimates at the observation sites are subtracted from the observations to generate *observation increments* or *observed-minus-background differences.* Next, the *analysis increments,* called *analysis-minus-background differences* or collectively as the *correction field,* are obtained by objective analysis of the observation increments. Then the analysis increment or correction field is added to the background estimate to obtain the final analysis.

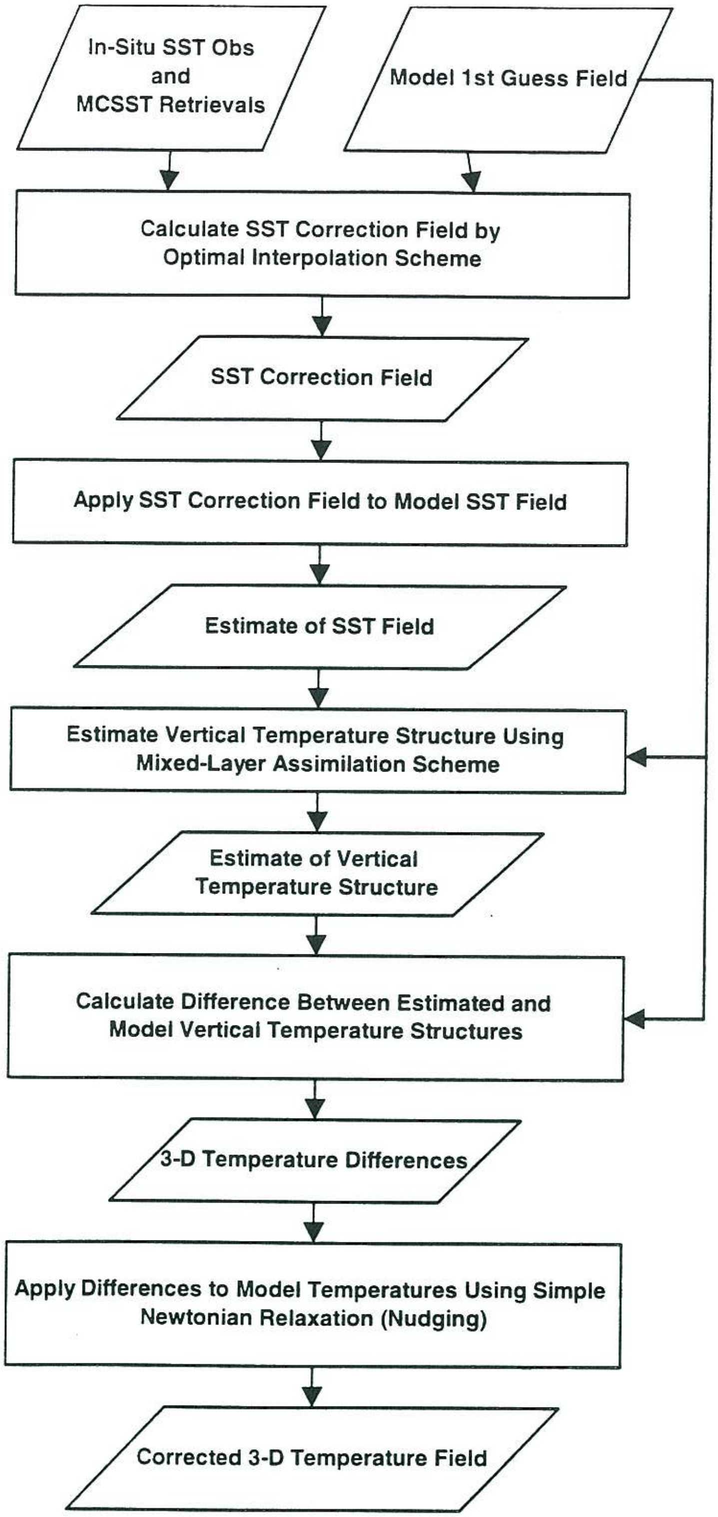

Figure 7. Flowchart depicting the steps of the COFS SST data assimilation system.

In the Derber-Behringer scheme the correction field is determined by *statistical interpolation* with the objective analysis equation solved using an equivalent variational formulation (Lorenc, 1986). The Derber-Behringer method seeks to combine model field and observations to estimate the correction field in a manner consistent with the estimated accuracy of each. This requires estimates of the spatial error covariances for the model and the observations. According to Derber and Rosati (1989), the variational formulation was chosen primarily because it eliminates costly and somewhat arbitrary data selection procedures. The formulation uses all observations in determining the correction field at each grid point.

1) Objective Analysis Function

In the variational framework, the goal is to minimize the objective function or functional. The objective function minimized in the Derber-Behringer approach consists of two terms. The first term is a measure of the fit of the corrected temperature field to the uncorrected model temperature field; and the second is a measure of the fit of the corrected temperature field to the observations. The solution is the correction temperature field which balances information from the observations with the model and its history (Behringer et al., 1998). The form of the functional is

$$I = \frac{1}{2}\mathbf{T}^{\mathbf{T}}\mathbf{E}^{-1}\mathbf{T} + \frac{1}{2}\left(\mathbf{D}(\mathbf{T}) - \mathbf{T}_{o}\right)^{\mathbf{T}}\mathbf{F}^{-1}\left(\mathbf{D}(\mathbf{T}) - \mathbf{T}_{o}\right) \tag{7.1}$$

where **T** is an N component vector of corrections to the model temperature field, **E** is an approximation to the N x N *model error covariance matrix*, $\mathbf{T}_o$ is an M component vector of differences between the observations and model temperatures, **D** is an interpolation operator from grid points to observation locations, and **F** is an approximation to the M x M *observational error covariance matrix*. The number of grid points is N and the number of observations is M. The transpose of the vector is indicated by $(\ )^T$ and the inverse of a matrix by $(\ )^{-1}$. The first term

$$\mathbf{T}^{\mathbf{T}}\mathbf{E}^{-1}\mathbf{T} \tag{7.2}$$

is a measure of the fit of the model or first guess weighted by the inverse of the first guess error covariance matrix to the corrected temperature field. The second term

$$(\mathbf{D}(\mathbf{T}) - \mathbf{T}_o)^T \mathbf{F}^{-1} (\mathbf{D}(\mathbf{T}) - \mathbf{T}_o) \quad (7.3)$$

is a fit of the observations weighted by the inverse of the observational error covariance matrix to the corrected temperature field. Thus for the first term, a larger error variance diminishes the contribution of the first guess to the final analysis, while for the second term, a relatively large error covariance diminishes the contribution of the observations.

2) Observational Error Covariance Matrix

As stated by Behringer (1994), error covariance matrices are poorly known and are specified in a simple ad hoc fashion. The observational error covariance matrix (**F**) is estimated only from measurement errors. No attempt is made to incorporate errors of representativeness. The measurement errors are treated as if they were uncorrelated and thus the matrix is diagonal (*i.e.* matrix's off-diagonal or non-diagonal terms are all zero). Since **F** is a diagonal matrix the inversion of **F**, $\mathbf{F}^{-1}$ can be defined directly. The initial estimates of the diagonal elements of $\mathbf{F}^{-1}$ are set to the reciprocal of an estimate of the *observational error variance.* Different estimates of the observational error variance can be assigned depending on data type. In the present version of the COFS assimilation system, the MCSST retrievals and SST observations are assigned the values given in Table 3.

Time is incorporated into **F** by the multiplication of the diagonal elements of $\mathbf{F}^{-1}$ by a *time factor.* In the current version of the COFS a time factor of 0.5 is assigned to yesterday's observations and 1.0 to today's observations. Thus, today's observations are given more weight.

A modification of the $\mathbf{F}^{-1}$ matrix can be applied when the magnitude of the temperature difference between the first guess field and the observations is greater than a specified minimum value (*e.g.* 8°C). For example, when the differences are between an arbitrary range of values (*e.g.* 8 – 16°C), the diagonals can be modified by the factor $1/[1+(|T_o|-5)^2]$ and thus given less weight. For differences greater than a specified maximum value (*e.g.* 16°C), the observations can be ignored and not used in the assimilation. This final modification acts as an additional quality control procedure. Presently, this modification is not active in the COFS assimilation.

3) First-Guess Error Covariance Matrix

The purpose of the objective analysis procedure is to spatially distribute the differences between the first-guess values and the observations, *i.e.* the observation increments. This is accomplished using the spatial structure of the first guess or error covariance, **E**. Thus, the first guess error covariance is considered the most important element in the data assimilation algorithm (Daley, 1991). In the Derber-Rosati scheme, **E** is defined so that the vertical correlations are ignored and the spatial correlations are assumed to be the same for each model level. In order to reduce computational costs, the horizontal covariances for a level are modeled by repeated applications of a *Laplacian smoother*. This results in a first-guess error covariance between any two points on a model layer that is approximated by

$$E(r) = a \bullet \exp\left(-\left(\frac{r}{b}\right)^2\right) \tag{7.4}$$

where a is the first guess error variance, r is the horizontal distance between two model grid points, b is the estimate of the correlation spatial or length scale of the model error. The first guess error variance, a, controls the relative weight between the observations and the first guess. Presently, a and b are set to arbitrary values of 0.50°C^2 and to 60 km, respectively.

The value of a could be determined by comparing model analysis with data. After making allowance for data error, the difference would provide an estimate of the first guess covariance. The value of a would then vary by geographical position. The value of *b* could be determined by finding the correlation scale of SST by subtracting the mean field, and finding the correlation scale of the variability. Like *a*, the value of *b* would then vary geographically.

4) Procedure to Minimize the Functional

The functional is minimized by using a preconditioned conjugate gradient algorithm. According to Derber and Rosati (1989), the algorithm does not attempt to directly find the minimum of the functional, but rather by iteration to find the solution. Formally, the conjugate gradient algorithm is defined as an iterative method for "unconstrained" minimization that produces a better approximation to the minimum of a general unconstrained nonlinear function of N variables, x_1, x_2, x_3,...x_N with each iteration (Navon and Legler, 1987), where N represents the number of variables of a discretized meteorological or oceanographic model. This type of algorithm generates directions of search without storing a matrix in contrast to other methods (Gill et al., 1981). A search direction is an estimate of the relative change to each initial grid point value to produce the maximum reduction in the functional; however, the search direction provides only the relative changes to the initial conditions, and not the absolute magnitude (Derber, 1987). The method is a good compromise between convergence rates and computer memory requirements (Navon and Legler, 1987). The algorithm performs the following basic steps:

1) test for convergence,
2) compute a *search direction*,
3) compute a *step size* or length, and
4) update the estimate for specifying the directions and then go back to step 1.

Specifically, Navon and Legler (1987) describe the conjugate-gradient algorithm in the following manner.

> "Within a given iteration an estimate is made of the best way to change each component of the vector x, so as to produce the maximum reduction of the function, by finding the gradient of the function with respect to the

> variables and combining this gradient with information from the previous iterations to produce a search direction. The search direction is an estimate of the relative change in each component of the vector x to produce the maximum reduction in the function F. To find the magnitude of the changes along the search direction, an optimal step size must be estimated. The new vector after an iteration, is given by the previous vector plus an optimal step size times the search direction."

The key quantities in the algorithm are 1) the derivative of the functional with respect to the correction field, **g** and 2) the term **h=Eg**. For the functional (7.1), the derivative **g** is given by

$$\mathbf{g} = \mathbf{E}^{-1}\mathbf{T} + \mathbf{D}^{\mathbf{T}}\mathbf{F}^{-1}\left(\mathbf{D}(\mathbf{T}) - \mathbf{T}_{\mathbf{o}}\right) \tag{7.5}$$

The term **g** is simplified by setting the precondition that the initial guess for the correction field, $\mathbf{T}^1$ be equal to zero. The equation for **g** is reduced to the following:

$$\mathbf{g} = -\mathbf{D}^{\mathbf{T}}\mathbf{F}^{-1}\mathbf{T}_{\mathbf{o}}\ . \tag{7.6}$$

This preconditioning allows the solution of the functional to be determined without directly inverting the first guess covariance **E** matrix.

The correction field is calculated through a series of iterations in the following sequence. First, the following search directions, **d** and **e** are calculated:

$$\mathbf{d}^{n} = -\mathbf{h}^{n} + \beta^{n-1}\mathbf{d}^{n-1} \tag{7.7}$$

and

$$\mathbf{e}^{n} = -\mathbf{g}^{n} + \beta^{n-1}\mathbf{e}^{n-1} \tag{7.8}$$

where n is the iteration counter, initially set to one, and β is a factor controlling the length of the previous search direction to be included in the current direction. Next, the value for **f** is determined by

$$\mathbf{f}^{n} = \mathbf{e}^{n} + \mathbf{D}^{\mathbf{T}}\mathbf{F}^{-1}\mathbf{D}\mathbf{d}^{n}. \tag{7.9}$$

The step size, α is calculated by

$$\alpha = \frac{\left(\mathbf{g}^{n}\right)^{1}\mathbf{h}^{n}}{\left(\mathbf{d}^{n}\right)\mathbf{f}^{n}}. \tag{7.10}$$

The derivative of the functional, **g** is determined by

$$\mathbf{g}^{n+1} = \mathbf{g}^{n} + \alpha^{n}\mathbf{f}^{n}. \tag{7.11}$$

The correction field is calculated by

$$\mathbf{T}^{n+1} = \mathbf{T}^{n} + \alpha^{n}\mathbf{d}^{n} \tag{7.12}$$

and **h** is determined according to

$$\mathbf{h}^{n+1} = \mathbf{E}\mathbf{g}^{n+1}. \tag{7.13}$$

The β term is estimated by

$$\beta^{n+1} = \frac{\left(\mathbf{g}^{n+1}\right)^{\mathbf{T}}\mathbf{h}^{n+1}}{\left(\mathbf{g}^{n}\right)^{\mathbf{T}}\mathbf{h}^{n}}. \tag{7.14}$$

Detailed discussions of conjugate gradient algorithms can be found in Gill et al. (1981) and Golub and VanLoan (1989).

5) Application of Scheme to COFS

The Derber/Behringer scheme has been adapted for use in COFS. In this section, a step-by-step description is given on how the scheme is executed in the model Fortran code, *pomcfs32n.f.*

Step 1: Read and Store SST Observation Records

The subroutine ESTCNT is called after the model restart file is opened and its contents read into arrays. The purpose of ESTCNT is to open and read the preprocessed SST data files and store their contents in arrays. The daily observation file contains sorted SST observation records within the COFS domain. Each record contains the name of the observing platform (RETRVL in the case of the retrievals), the date and time of the observation, the latitude and longitude and decimal I and J model coordinates of the observations. ESTCNT also attaches the integer -1 when the record is for 'yesterday'. ESTCNT is called a second time to read and store SST observation records for 'today' and to assign the integer value 0 to each record.

Step 2: Calculate Normalization Weights

The subroutine IASSIM is called after the second call to subroutine ESTCNT. The first task of IASSIM is to assign values to *acoef* (*a* in equation 7.4). The parameter *acoef* is the model first guess covariance which is an assignment of the relative weight between the observations and the model fields and is constant over the entire model grid. The second task is to assign a value to *bb(1)*, which is the constant defining the spatial scale of the Gaussian function. The constant *bb* is related to *b* in equation 7.4 in the following manner:

$$bb = (0.5 * b)^2. \tag{7.15}$$

The constants *acoef* and *bb* are presently set to 0.5°C^2 and 900.0 km^2 (since *b* is assigned a value of 60 km), respectively. Next, IASSIM calls subroutine XXCON to calculate the normalization weights or factors. These weights are needed later by subroutine LPSMTH. Subroutine XXCON calculates the weights by applying the Laplacian smoother to a unit "correction" at each grid point. The calculation of the weights takes into account the varying horizontal resolution of the COFS grid by using the varying DX and DY grid increments. Near the end of subroutine IASSIM, the square root is taken of the weights according to

$$wgta = \sqrt{\frac{acoef}{wgns}}. \tag{7.16}$$

This is done to renormalize the weights and to prepare the weights for the two applications of the smoother in subroutine LPSMTH. The weights ensure that the diagonal elements of the equivalent **E** matrix are equal to *acoef*.

Step 3: Calculate Initial Values for **g** and **h**

The subroutine ASSIM is called in the main section of the *pomcfs32n.f* within the DO 9000 Loop,*i.e.* the internal mode loop, every time step 720 seconds (0.2 hours).

Experiments are being conducted to determine if the assimilation can be done less frequently, i.e. 1 or 3 hour intervals.

The subroutine performs a series of tasks. These tasks are accomplished within the subroutine and via calls to other data assimilation-related subroutines including COMOBS and DTFDI.

The first task is to call subroutine COMOBS to combine SST records for yesterday and today into a common array. The records are combined row by row from south to north. Next, IASSIM initializes the search directions, $\mathbf{d}^{o}$ and $\mathbf{e}^{o}$ to zero. In addition, the initial guess for the correction field, $\mathbf{T}^{1}$ is set to zero.

The third task is a call to subroutine DTFDI for each row of COFS grid except the first and last. This subroutine performs the following tasks:

1) bilinearly interpolates the model values to observation locations,

2) determines the observation increments by calculating the difference between the observations and model values at the observation sites,

3) eliminates observations which differ from model temperature values by greater than a user specified amount, if required by user, and

4) calculates the initial value of the derivative of the functional with respect to the correction field (see equation 7.6).

Near the end of COMOBS, **g** is stored in a 3-D array called *ares*. This array is first used in the subroutine LPSMTH.

The fourth task is a call to subroutine LPSMTH. The purposes of this subroutine are to

1) calculate an initial value of **h** by multiplying the initial value of the functional **g** by an approximation to the first-guess error covariance matrix, **E** (equation 7.13), and

2) calculate the inner product, $(\mathbf{g})^{T}\,\mathbf{h}$ (*ghip*).

As mentioned earlier, the approximation to **E** is determined by the application of the Laplacian smoother using the weights calculated earlier in XXCON and IASSIM.

Step 4: Perform Iterations

The forth-major step is the iterations of the conjugate gradient algorithm. This is done in subroutine ASSIM and involves subroutines DTFD, GMAT, and LPSMTH. First, the search directions **e** (*dir*) and **d** (*edir*) are calculated by a call to subroutine GMAT. In addition, GMAT calculates the inner product, $(\mathbf{d})^T \mathbf{f}$ (*dfip*) after a call to DTFD to determine the second term in equation 7.9. Then back in ASSIM, the step size α (*astep*) is calculated according to equation 7.10. The step size is restricted to values greater than or equal to one. Next, new values of **g** and **T** (*ecor*) are calculated, followed by a call to LPSMTH to determine a new value of **h** (*ghip*). Then, ASSIM calculates a new value for β (*cbeta*) which is the parameter controlling the amount of previous search direction to be included in the current direction. The later is based on the present and previous values of the inner product, $(\mathbf{g})^T\mathbf{h}$.

Step 5: Calculate Correction Field

The last step is to calculate the final correction field, **T** (*ares*), with equation 7.13. This is done at the end of the subroutine ASSIM by

```
ARES(:,:,j)=ECOR+ASTEP * EDIR.
```

The correction field is then added to the model simulated SST field (*TB*) in the main section of *pomcfs32n.f* to obtain the final analysis for the model's top layer temperature. An example of the SST correction field is given in Fig. 8.

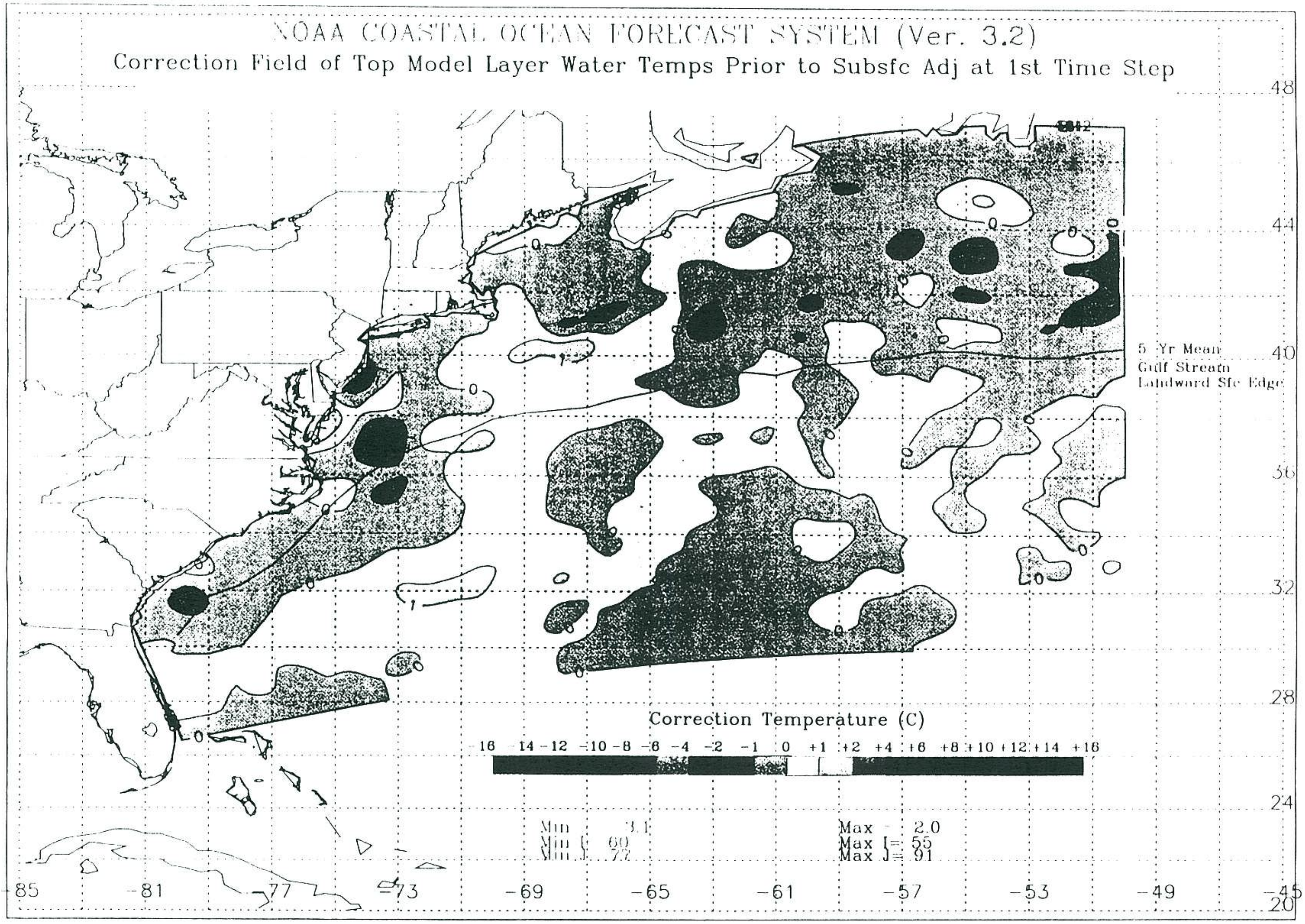

Figure 8. An example of a COFS SST correction field.

b) Mixed Layer Assimilation Procedure

The corrected top layer temperature field serves as the target for a mixed-layer extrapolation scheme (Chalikov et al., 1996) to estimate a new subsurface temperature structure down through the mixed layer. The scheme is similar to the one used by the ocean data assimilation system of the United Kingdom Meteorological Office's Forecasting Ocean Atmosphere Model (Forbes, 1995). Both schemes rely on the fact that the surface water temperature is well correlated with the temperature of the mixed layer.

The Chalikov scheme checks to see whether the corrected surface temperature field is warmer or cooler than the model's first guess. When the corrected field is warmer than the first guess, the surface temperature difference is distributed throughout the mixed-layer. When the corrected field is colder than the first guess, the corrected field replaces the model temperatures down to the depth where they become equal.

Step 1: Calculate Depth of Mixed Layer

The first step determines the depth of the mixed layer. The location is estimated from the model's temperature field, i.e. TB variable, in the following manner. At each grid point the temperature gradient (°C m^{-1}) between adjacent layers is calculated using the actual vertical distance between layers. The depth of each sigma layer is calculated by multiplying H, the ocean depth (m), by ZZ(K), the nondimensional depth of the sigma. The location and value of the maximum gradient at each grid point is stored in KMXLAY(I,J) and GRADMAX(I,J), respectively. The depth of the maximum temperature gradient is stored in DEPMAX(I,J). As noted by Forbes (1995), the mixed layer depth is a diagnostic calculated from the model thermal field which may contain errors.

Step 2: Calculate New Temperature Profile

The next step estimates a new temperature profile depending on whether the assimilated SST, ASMSST(I,J) is greater or smaller than the non-corrected SST, ORGTB (I,J,1). When ASMSST(I,J) > ORGTB(I,J,K), then the surface difference is distributed throughout the mixed-layer up to an maximum depth of 200 m. This is accomplished in the following manner. First, the difference between the corrected surface field and original model temperature at the bottom of the mixed layer is calculated by

DIFFS= (ASMSST(I,J)-ORGTB(I,J,KHM)),

where KHM is the k index of the sigma layer of the bottom of the mixed layer. Next, the difference between the original model SST and original model temperature at the bottom of the mixed layer is calculated by

DTMLYS=(ORGTB(I,J,1)-ORGTB(I,J,KHM)).

Next, a non-dimensional temperature profile is calculated by

XNDTP=MAX(0.0,MIN(1.0,DTMLYS/DTMIXL)),

where XNDTP is constrained to be between 0 and 1. Finally, a new temperature profile is calculated by distributing the difference between the model and observed SST proportional to the non-dimensional temperature profile. This is done by the statement

ASM2TB(I,J)=ORGTB(I,J,KHM)+DIFFS*XNDTP.

When ASMSST(I,J) is less than or equal to ORGTB(I,J,1), then ASMSST(I,J) values are assigned to ASMT2B(I,J,K) down to the depth where they become equal.

Step 3: Calculate Difference Between Original and New Temperature Profile

The third step computes the difference between ASM2TB, the new temperature profile, and ORGTB, the original temperature profile following mixed layer assimilation. This value is stored in TDDIF(I,J,K).

c) Nudging

This difference (TDDIF or FFDIF) is applied to the model TB field over time by Newtonian relaxation or nudging. Nudging is a method in which model variables are driven toward observations by extra forcing terms in the model equations (Haltiner and Williams, 1980). It is assumed that the time rate of change of TDDIF is proportional to the present temperature difference. The application of this difference is accomplished in POM's standard subroutine ADVT, the horizontal scalar advection subroutine. This subroutine uses the leap frog time method to calculate the temperature at the forward time step.

The temperature difference TDDIF(I,J,K) is distributed over the length of the model run by the statement:

```
DIFAMT=FFDIF(I,J,K)*GAMMA,
```

where FFDIF is the difference between the present estimated profile and the previous model profile (calculated as TDDIF in the subroutine MIXASM), and GAMMA is a constant of proportionality. It is set to 10^{-4}, an order of magnitude less than 1/DTI. Thus, the temperature difference applied to the model decreases as time increases.

The temperature difference is applied in the leap frog statement:

```
FF(I,J,K)=(FB(I,J,K)*(H(I,J)+ETB(I,J,K)*ART(I,J)-

          DTI2*FF(I,J,K))/((H(I,J)+ETF(I,J))*ART(I,J)) + DIFAMT
```

where FF and FB are the calculated temperatures at forward and previous time steps, H is the bottom depth (m), ETB is the surface elevation (m) at the back time step, ETF is the surface elevation (m) at the forward time step, ART is the area of a grid box centered at a depth point (m), and DTI2 is twice the internal mode (baroclinic) time step.

8.0 POTENTIAL IMPROVEMENTS

Potential improvements to COFS include the following:

1) Perform data assimilation at less frequent intervals (e.g. every hour).

2) A new version of the COFS data assimilation cycle is being tested which uses 3 hourly analyzed fields from EDAS as a replacement to the Eta forecast fields. If successful, the COFS data assimilation cycle will use analyzed fields from EDAS and the COFS forecast cycle will use forecast fields from the Eta-32 model.

3) Another version of COFS is being run which assimilates satellite-derived altimetry data from the Topex/Poseidon satellite. This version will replace COFS 3.2 as the semi-operational version.

4) Additional quality control procedures for SST observations such as checks for geographic positional errors.

5) The assimilation of MCSST retrievals from GOES into COFS.

6) Run COFS twice a day with forecasts out to 48 hours or longer.

7) Run COFS with surface forcing from NCEP's Aviation Model as backup.

8) Use near real-time USGS river observations and NWS river forecasts.

9) Run COFS on NCEP's SGI Origin 2000 workstation and IBM SP computer.

10) Modify COFS programs to be Y2K compliant.

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