Retrospective Air Quality Simulations of the TexAQS-II: Focused on Emissions Uncertainty

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ABSTRACT

There are several studies on the effects of emissions of highly reactive volatile organic compounds (HRVOC) from the industrial sources in the Houston-Galveston-Brazoria (HGB) area on the high ozone events during the Texas Air Quality Study (TexAQS) in summer of 2000. They showed that the modeled atmosphere lacked reactivity to produce the observed high ozone event and suggested “imputation” of HRVOC emissions from the base inventory. Byun et al. (2007b) showed the imputed inventory leads to too high ethylene concentrations compared to the measurements at the chemical super sites but still too little aloft compared to the NOAA aircraft. The paper suggested that the lack of reactivity in the modeled Houston atmosphere must be corrected by targeted, and sometimes of episodic, increase of HRVOC emissions from the large sources such as flares in the Houston Ship Channel (HSC) distributed into the deeper level of the boundary layer. We performed retrospective meteorological and air quality modeling to achieve better air quality prediction of ozone by comparison with various chemical and meteorological measurements during the Texas Air Quality Study periods in August-September 2006 (TexAQS-II). After identifying several shortcomings of the forecast meteorological simulations and emissions inputs, we prepared new retrospective meteorological simulations and updated emissions inputs. We utilized assimilated MM5 inputs to achieve better meteorological simulations (detailed description of MM5 assimilation can be found in F. Ngan et al., 2012) and used them in this study for air quality simulations. Using the better predicted meteorological results, we focused on the emissions uncertainty in order to capture high peak ozone which occasionally happens in the HGB area. We described how the ozone predictions are affected by emissions uncertainty in the air quality simulations utilizing different emission inventories and adjustments.

Key words: TexAQS-II, Emissions uncertainty, Houston ozone, HRVOC, CMAQ

1. INTRODUCTION

Currently, the Houston-Galveston-Brazoria (HGB) area is classified as a severe ozone nonattainment area. The region must reduce its ozone levels through an effective State Implementation Plan (SIP) to comply with the US Environmental Protection Agency (US EPA) standards as specified in the Clean Air Act and its Amendments. Air quality models are used to guide the development of air quality regulations and standards and to create SIP for managing air emissions. Accurate meteorological and photochemical modeling results are essential to support the efforts for establishing SIP by the local government such as Texas Commission on Environmental Quality (TCEQ). To provide routine air quality forecasting (AQF) and to support the 2006 Second Texas Air Quality Study (TexAQS-II), University of Houston operated the East Texas Air Quality (ETAQ) forecasting system. We performed daily operation of two-day air quality forecasting simulations at the 12-km resolution for the Eastern Texas regional domain and at the 4-km resolution for the HGB domain. Byun et al. (2007a) provided a detailed performance evaluation of the 2005/2006 ETAQ forecasting system. It showed that the AQF systems were capable of forecasting day-to-day ozone variations in East Texas and showed good performance in predicting averaged (either spatially, temporally or both) ozone. However, we found a few air quality simulation errors that could have been caused by the imperfect meteorology forecasting as well as the emissions inputs.

There are several studies on the effects of emissions of highly reactive volatile organic compounds (HRVOC) from the industrial sources in the HGB area on the high ozone events during the Texas Air Quality...
Study (TexAQS) in summer of 2000 (Murphy and Allen, 2005; Daum et al., 2004; Rayerson et al., 2003). They showed that the modeled atmosphere lacked reactivity to produce the observed high ozone event and suggested “imputation” of HRVOC emissions from the base inventory (i.e., selectively increasing ethylene emissions by up to factor 21, and on the average 160–200 tons per day). Byun et al. (2007b) showed the imputed inventory leads to too high ethylene concentrations compared to the measurements at the chemical super sites but still too little aloft compared to the NOAA aircraft. The paper suggested that the lack of reactivity in the modeled Houston atmosphere must be corrected by targeted, and sometimes of episodic, increase of HRVOC emissions from the large sources such as flares in the Houston Ship Channel (HSC) distributed into the deeper level of the boundary layer.

We performed retrospective meteorological and air quality modeling to achieve better air quality prediction of ozone by comparison with various chemical and meteorological measurements during the Texas Air Quality Study periods in August-September 2006 (TexAQS-II). After identifying several shortcomings of the forecast meteorological simulations and emissions inputs, we prepared new retrospective meteorological simulations and updated emissions inputs. We utilized assimilated MM5 inputs to achieve better meteorological simulations (detailed description of MM5 assimilation can be found in N. Ngan et al., 2012) and used them in this study for air quality simulations. Using the better predicted meteorological results, we focused on the emissions uncertainty in order to capture high peak ozone which occasionally happens in the HGB area. We described how the ozone predictions are affected by emissions uncertainty in the air quality simulations utilizing different emission inventories and adjustments.

2. METHODOLOGY

2.1 MM5-SMOKE-CMAQ Modeling System

The air quality modeling system used in this study is the Environmental Protection Agency (EPA)'s Community Multiscale Air Quality (CMAQ) (Byun and Schere, 2006; Byun and Ching, 1999) modeling system. The primary modeling components in the CMAQ modeling system include: (1) Penn State-NCAR Fifth generation Mesoscale Model (MM5) (Grell et al., 1994) meteorological modeling system for the description of atmospheric states and motions; (2) Sparse Matrix Operating Kernel for Emissions (SMOKE) models for processing man-made and natural emissions that are injected into the atmosphere; and (3) CMAQ Chemistry Transport Modeling (CTM) system for the simulation of chemical transformations and fate of emissions.

The modeling domain was defined with the Lambert Conformal Conic map projection with the first true latitude (alpha) at 30°N, second true latitude (beta) at 60°N, central longitude (gamma) at 100°W, and the projection origin at (100°W, 40°N). The spheroid used is a perfect sphere with a radius of 6,370.997 meters. The MM5 simulations for the Eastern Texas area were conducted for three domains at different horizontal resolutions (36-, 12- and 4-km) and 43 variable vertical layers with one-way nesting. CMAQ domains at different resolutions were subsets of the respective meteorological modeling domains. For the CMAQ simulations we kept the same vertical layer structure as MM5 for the lower 12 layers (i.e., ~1 km) but upper 33 layers of MM5 were collapsed to form 11 CMAQ layers to reduce computation cost. The thickness of lowest model layer was ~34 m.

2.2 Preparation of Emissions Data

2.2.1 Base-case AQF Emissions Inputs

Air quality forecasting utilizing the MM5-SMOKE-CMAQ system has been operating in the University of Houston since May 2005. The emissions for air quality forecasting were processed using the Texas emissions inventory (TEI) for base year 2000 which is projected to year 2005 utilizing growth and control factors (TCEQ, 2008a). The emissions inputs for the air quality forecasting system have been used as the base-case emissions in this study. Based on TexAQS 2000 aircraft measurements and VOC reactivity analysis of gas chromatography observations at a few surface sites Ryerson et al. (2003) and Wert et al. (2003) suggested serious underprediction of HRVOC emissions in the inventories. In response to this TCEQ selectively increased HRVOC emissions from the regular inventory values and generated “imputed” HRVOC emissions for year 2000 (Byun et al., 2007b). The additional volatile organic compounds (VOC) emissions increased from non-electric generation utilities over the HGB area amount to ~170 tons/day while total VOC emissions in the regular emissions inventory are ~230 tons/day from the area. To represent the impact of the imputed VOC emissions in the air quality simulations, they were used without projection to approximate industrial emissions in the Houston Ship Channel. For biogenic emissions, vegetation data from TCEQ was used and then adjusted with the Meteorology-Chemistry Interface Processor (MCIP)-processed meteorological data. More detailed descriptions of the AQF emissions can be found from the Houston Advanced
Research Center (HARC) project final report on East Texas Air Quality (ETAQ) Forecasting (Byun et al., 2007a).

2. 2. 2 Best-effort Model Ready 2006 Emissions Inputs

In addition to air quality simulations using the base-case AQF emissions, we decided to prepare “best-effort model-ready (BEMR) 2006 Texas emissions inputs” utilizing currently available emissions inventories to perform air quality simulations for the assessment study and to see how different emissions inputs affect air quality simulations during summer 2006. Compared to the base-case AQF emissions, the BEMR emissions include major revisions in point and mobile emission inventories. First, the BEMR emissions inputs include the 2006 special point source emission inventories for summer 2006 TexAQS II (TCEQ, 2008b) in which a set of hourly-specific, and speciated VOC and NOx emissions from point sources are estimated. Total point source VOC emissions in the BEMR emissions are around 210 tons/day for the HGB area, similar to the total point source VOC emissions in the 2000 regular inventory (~230 tons/day) but shorter than the base-case AQF when the additional VOC emissions are applied. Secondly, the MOBILE6 emissions estimated for year 2003 were used in the base-case AQF emissions, while the MOBILE6 emissions for 2005 were used for the BEMR emissions. Note that ~20 tons of nitrogen oxides (NOx) emissions from mobile sources decreases every year for the HGB area according to the emissions estimated. Table 1 summarizes the differences of inventories between AQF emissions and BEMR emissions.

|                      | Base AQF | BEMR        |
|----------------------|----------|-------------|
| Area & Non-road      | Base year 2000 | Base year 2007 |
| On-road              | MOBILE6 for year 2003 | MOBILE6 for year 2005 |
| Point                | Regular emissions projected for 2005 & additional VOC for 2000 imputation | 2006 Texas point-source special inventory (TPSI2006) |
| Biogenic             | Old vegetation data from TCEQ | New vegetation data from TCEQ |
| Supplementary        | NEI99    | NEI2002     |

Table 1. Emissions inventories used for the base AQF and the “best-effort model-ready” (BEMR) Texas Emission Inputs.

3. RESULTS AND DISCUSSION

3.1 Comparison of the Base AQF and the Updated BEMR Emissions Inputs

Fig. 1(a), (b), and (c) compares NOx, VOC, and carbon monoxide (CO) emissions for the HGB area estimated for the AQF and BEMR emissions. It is noted that not only VOC emissions but also NOx emissions from point sources reduce almost by half when the 2006 special point source emissions are used in the BEMR emissions for the region. Mobile VOC emissions in the BEMR emissions decrease by ~15%, cor-
responding to the reduced NOx emissions when compared to the AQF emissions. For non-road mobile sources, about 30% of VOC emissions reduce in the BEMR emissions, but NOx emissions from the sources are almost the same. In case of area sources, similar NOx emissions are estimated while VOC emis-

Fig. 2. Comparison of hourly emissions rates of (a) NO, (b) CO, (c) OLE, and (d) ETH between the base and updated emissions for the HGB 8-county area during the August 15-September 14, 2006. Purple and orange lines represent the base AQF (denoted as “AQF”) and updated BEMR 2006 (denoted as “BEMR”) emissions, respectively.
isons in the BEMR increase by 10% compared to the AQF emissions. Thus, overall VOC/NOx emission ratios from all the sources for the area remain almost the same when VOC and NOx emissions in the BEMR emissions reduce more than 200 tons/day and around 350 tons/day, respectively, compared to the AQF emissions. Fig. 1(c) presents that the CO emissions in the BEMR emissions decrease from mobile, nonroad, and point sources and reduce by ~10% compared to the AQF emissions. Fig. 1(d) shows the HRVOC (ethylene (ETH), olefin (OLE)) and formaldehyde (FORM) emissions, which are estimated after chemical speciation by SMOKE processing, in the AQF and BEMR emissions. Note that the unit is Mmole per day. ETH and OLE emissions in the BEMR emissions decreased by ~75% and 70%, respectively, compared to the AQF emissions. FORM emissions are slightly reduced in the BEMR emissions.

Fig. 2(a) and (b) show that nitrogen oxide (NO) and CO emissions rates in the HGB 8 counties (Brazoria, Chambers, Fort Bend, Galveston, Harris, Liberty, Montgomery, and Waller). The updated BEMR emissions are reduced by 30-35% for NO and 10-15% for CO, compared to the base AQF emissions. It should be noted that in addition to the use of 2006 point special inventory, the updated BEMR emissions data include mobile emissions projected for 2005. Because the base AQF emissions data uses MOBILE6 emissions projected for 2003, the BEMR NOx and CO emissions are lower than the corresponding base AQF emissions. In Fig. 2(c) and 2(d), olefin (OLE) and ethylene (ETH) emissions rates in the HGB 8 counties are presented. The updated BEMR emissions are reduced by 25% for OLE and 40% for ETH, compared to the base AQF emissions. No imputation is applied to the updated BEMR point-source special inventory, while additional imputed VOC emissions (~170 tons/day) are used for the base AQF emissions. Note that early morning peaks in ETH emissions that are repeated for the week days (Monday-Thursday) in the base AQF emissions data are absent in the updated BEMR emissions data (Fig. 2(d)). These peaks were originally present in the 2000 daily imputed ethylene inventory.

3.2 Comparison of CMAQ Simulations with the Base AQF and the BEMR Emissions Inputs

It should be first noted that we used assimilated MM5 inputs for CMAQ simulations to provide better meteorological field. Details on how we assimilated MM5 with observations can be found in F. Ngan et al. (2012). The Continuous Ambient Monitoring Stations (CAMS) sites utilized for the evaluation are shown in Fig. 3.

![Fig. 3. Locations of CAMS sites (circle) in the HGB area used in the analysis.](image)

We compared the results of a CMAQ simulation using the “best-effort model-ready” (BEMR) emissions to those from a CMAQ simulation using the base AQF emissions. Both simulations utilized the assimilated MM5 inputs (denoted as “RS_m”). During this process, we found several quality assurance issues with the newly prepared emissions, and the final simulation set used here was named as the “retrospective simulation with the assimilated meteorology and updated emission inputs” (denoted as “RS_m++e”). For identification purposes, the two simulations are referred to as follows:

(a) RS_m: assimilated meteorology (RS_m)+AQF emissions
(b) RS_m++e: assimilated meteorology (RS_m)+BEMR emissions

The regional average NO and NO2 time series plot is presented in Fig. 4(a) and (b). It revealed a general underprediction of NO at early morning hours and overprediction of NO2 for the nighttime and early morning hours. NO frequently dropped almost zero at early night (before midnight), resulting in no more ozone titration after that time. This can be one of the reasons for the high bias of ozone at nighttime and suggest a need to impute or reconcile NO emissions. The morning high peaks in both NO and NO2 was possibly related to misrepresentation of morning PBL growth. ETH simulations (Fig. 4(c)) with AQF emissions seriously overpredicted ETH concentration for nighttime and early morning and somewhat overpredicted during daytime hours, while with BEMR emissions match better with observations.
The regional average ozone time series plot is presented in Fig. 4(d). Emission input changes, although substantial, did not result in large changes. In general, the “RS_m+e” simulations show lower ozone peak concentrations than the “RS_m” simulations. The former simulates lower ozone days better than the latter, but is worse when simulating peak ozone events. Scatter plots comparing simulated hourly ozone and corre-

Fig. 4. Time series plot of (a) NO, (b) NO₂, (c) ETH, and (d) ozone averaged over the CAMS sites in the HGB area for the August 30-September 5, 2006 period.

Fig. 5. Scatter plots of model (RS_m=left, RS_m+e=right) simulated ozone versus CAMS observations in the HGB area for the August 30-September 5, 2006. All hourly data pairs in the HGB area are used for the comparison.
sponding CAMS observations from August 30 to September 5 are presented in Fig. 5. Statistical values of RS$_m$++ case were slightly better than those of RS$_m$ case. Correlation coefficient improved from 0.685 to 0.705 and root mean square error reduced from 25.7 to 21.5. Simulations with the BEMR emissions (RS$_m$++) show slightly less scatter than those with the base AQF emissions (RS$_m$). However, RS$_m$++ case fails to predict ozone peaks over 120 ppb.

To investigate the more detailed impact of using different emissions, we compared model results with two specific CAMS sites and University of Houston (UH) Moody Tower super site. The Lynchburg Ferry site, which is located in the coastal area of the Houston Ship Channel, often represents complex meteorological changes due to the influence of Galveston Bay and large nearby emissions sources on air quality. The model often severely overpredicts ETH (Fig. 6(a)) with the imputed HRVOC emissions (RS$_m$ case) in the evening and during the night, while it somewhat underpredicts with the BEMR emissions (RS$_m$++ case). Although HRVOC imputed emissions inputs generate higher ozone concentrations than the BEMR emissions, both simulations failed to produce high peak ozone during the episode days (for example, August 31 and September 1) and the underprediction of peak ozone is much bigger in the simulation case with BEMR emissions (RS$_m$++) as shown in Fig. 6(b).

The HRM-3 site is one of the important Houston Regional Monitoring (HRM) networks for monitoring air quality in the Houston Ship Channel. ETH simulations (Fig. 6(c)) with the BEMR emissions (RS$_m$++) match well with observations although on some days it fails to reach observed peak values. On the other hand, the simulations with base AQF emissions (RS$_m$) overpredict ETH by a factor of 4 or more, even during daytime hours. The predicted peak ozone concentrations with the AQF emissions are higher than those with the BEMR but not by much considering the significant difference in the emissions inputs used (Fig. 6(d)). Similar to Lynchburg Ferry site, both simulations failed to produce high peak ozone during the episode days.

The model simulation results are also compared with measurements made at the UH Moody Tower super site (60 m above ground level, corresponding to model second layer) (Fig. 7). The ETH concentrations predicted with the AQF emissions are much higher compared with observation, while those with the BEMR emissions show somewhat underpredictions in the morning hours but without large discrepancies during daytime hours. The discrepancy in the simulated ETH
3.3 Sensitivity of CMAQ Results to Adjusted BEMR Emissions

For the TCEQ special inventory for 2006, Cuclis (2009) indicated that measured levels of ethylene and propylene were higher than expected from the inventory by a factor of 10 or more. It is also suggested in the TCEQ report (TCEQ, 2007) that mobile emission inventories developed from MOBILE6 consistently overestimates CO emissions by at least a factor of 2 and underestimates NOx emissions in the HGB area. Based on these suggestions, we increased OLE (olefinic carbon bond species), which is lumped species in the CB-4 mechanism and more reactive than ethylene, emissions in the Houston Ship Channel area as well as mobile NOx emissions in the HGB area, and decreased mobile CO emissions in the HGB area to improve CMAQ simulations. Detailed amount of the adjusted BEMR emissions are as follows:

(a) Point source OLE emission in the Houston Ship Channel area.
(b) Increased mobile NOx emissions in the HGB area.
(c) Decreased mobile CO emissions in the HGB area.

Fig. 7. Time series plot of (a) ETH, (b) NOx (NO + NO2), (c) CO, and (d) ozone concentration at the UH Moody Tower for the August 30-September 5, 2006 period.

Fig. 8. Locations and identification number of CAMS sites (circle) in the Houston area. Gray circles indicate the CAMS sites located in the Houston urban area (Red=Houston Ship Channel, Green=north downwind urban, Pink=south downwind urban, Blue sites are not used in the analysis).
Channel by 12 times for layers 1-5
(b) Mobile source NOx emissions in the HGB area by 1.5 times
(c) Mobile source CO emissions in the HGB area by 0.5 times

After adjustments of BEMR emissions, we focused on two days (August 31 and September 1) when ozone episode occurred in the HGB area in order to see how much emissions adjustments affect on CMAQ ozone predictions. We, then, compared the results of CMAQ simulations using the adjusted BEMR emissions to those from CMAQ simulations using the BEMR emissions. For identification purposes, the two simulations are referred to as follows:

(a) RS_m+e: assimilated meteorology (RS_m)+ BEMR emissions
(b) RS_m+e_adjusted: assimilated meteorology (RS_m)+adjusted BEMR emissions

For the detailed analysis, we divided the Houston area into several sectors as shown in Fig. 8.

The regional average of Houston Ship Channel and Houston Urban area for CO and NOx time series plots are presented in Fig. 9. The change in CO (50% reduction) and NOx (50% increase) emissions resulted in slight decrease of CO and increase of NOx concentration during daytime hours. The large differences between the two model results are found in the morning rush hours when the CO and NOx emissions from vehicles are trapped within the relatively stable atmosphere before the PBL evolution. Fig. 10 shows the simulation results at the UH Moody Tower which is located in the Houston urban area on the left-hand side of Houston Ship Channel. Similar to CO and NOx differences at the surface measurement sites, slight differences are made during daytime hours and large differences are found in the morning at the UH Moody Tower (Fig. 10(a) and (b)). As expected, ETH concentration of two simulations is almost identical because we did not adjust ETH emissions (Fig. 10(c)). Formaldehyde (HCHO) is the most abundant aldehyde in the atmosphere and contributes to further ozone formation. The main primary source of HCHO is the direct emission from incomplete combustion processes such as vehicles and the main secondary source of HCHO is the oxidation of hydrocarbons. Since we adjusted OLE in the Houston Ship Channel only, the differences between the two simulations represent the secondary HCHO. The HCHO concentration differences of the
two model results are made when the winds are blown from the east and the maximum differences are found on August 31 in the morning hours due to combination of easterly winds blown from the Houston Ship Channel and relatively shallow mixing height at the site (Fig. 10(d)).

Spatial changes in the ozone concentration due to adjusted emissions are presented in Fig. 11. It shows that increase of emissions resulted in higher ozone concentration, which is closer to observation, in the

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**Fig. 10.** Time series plot of (a) CO, (b) NOx, (c) ETH, and (d) Formaldehyde (HCHO) concentration at the UH Moody Tower for the August 31-September 1, 2006 period.

**Fig. 11.** Spatial ozone plots for the simulation with BEMR emissions (left) and adjusted BEMR emission (right) at 2006.09.01:15 CST. Model simulated winds (arrow) and CAMS observations (circle) are overlaid on the plot.
Fig. 12. Time series plots of regional average ozone concentration in the (a) HSC, urban, downwind urban (north, west, and south), (b) HSC, (c) Houston urban, (d) west downwind urban area for August 31-September 1, 2006.

Fig. 13. Scatter diagrams of ozone predicted by CMAQ with BEMR emissions (left) and adjusted BEMR emissions compared with CAMS observations in the HSC, urban, downwind urban (north, west, and south) area for the August 31-September 1, 2006 period. Daytime hourly data pairs are used for the comparison.
Houston Ship Channel area as well as west and north-west downwind urban area. The regional averaged model results corresponding to CAMS locations shows that peak ozone concentrations are increased by 10-20 ppb due to adjustment and match better with observed peak ozone (Fig. 12). There, however, are still underprediction of peak ozone in the west downwind urban area on August 31 and Houston Ship Channel area on September 1. It should be noted that the adjusted emissions not only increase peak ozone during daytime but also slightly decrease high bias during nighttime. Scatter diagram in Fig. 13 also support that the CMAQ with adjusted BEMR emissions can produce high peak ozone on event days, while CMAQ with BEMR emissions can not produce ozone values higher than 120 ppb when observed ozone values are over 120 ppb.

4. CONCLUSIONS

Houston suffers from serious ozone air quality problems due to emissions from the Houston metropolitan traffic and various petrochemical industrial facilities located around the Houston Ship Channel. The ozone precursor emissions interact with meteorological conditions determined by the complex coastal geographical features of the HGB region creating a unique environment for the development of high ozone.

Air quality simulations for the TexAQS-II in summer 2006 were conducted with two different emission inputs. To generate better emission inputs for modeling, we processed the updated 2006 Texas point-source special inventories to generate the “best-effort model ready” (BEMR) emissions. The results were compared with the base AQF emissions for year 2005 that included the additional year 2000 “imputed” volatile organic compound (VOC) emissions of ~170 tons/day. CMAQ simulations showed that the imputed AQF emissions seriously overpredicted precursor HRVOC concentrations while the BEMR underpredicted them. The regional average NO and NO2 time series plots show a general underprediction of NO at early morning hours and overprediction of NO2 for the nighttime and early morning hours. Although emission input changes did not result in large changes of CAMQ ozone prediction, CMAQ with BEMR emissions simulates lower ozone days better than the CAMQ with AQF emission but is worse when simulating peak ozone events.

Based on the other researches, we adjusted BEMR emissions of OLE from point sources as well as NOx and CO from mobile sources. The change in CO (50% reduction) and NOx (50% increase) emissions resulted in slight decrease of CO and increase of NOx concentration during daytime hours. CMAQ with adjusted BEMR emissions resulted in higher ozone concentration, which is closer to observation, in the Houston Ship Channel area as well as west and north-west downwind urban area. The regional averaged model results corresponding to CAMS locations shows that peak ozone concentrations were increased by 10-20 ppb due to adjustment and matched better with observed peak ozone.

We described how the CMAQ ozone predictions are affected by emissions uncertainty in the HBG area utilizing different emission inventories and adjustments. Through these analyses, we could suggest that the updated TPSI2006 inventories underestimates HRVOC emissions emitted from Houston Ship Channel, although the uncertainties in the Ship Channel industries were reduced compared to the 2000 case.

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