

PREDICTIONS OF NORTH AMERICAN BACKGROUND OZONE IN TEXAS

Elena McDonald-Buller*, Yosuke Kimura, Gary McGaughey, and David T. Allen
Center for Energy and Environmental Resources, University of Texas at Austin, Austin, TX, USA

Melissa Sulprizio and Daniel Jacob
Harvard University, Cambridge, MA, USA

Jaegun Jung, Greg Yarwood, Jeremiah Johnson, and Chris Emery
ENVIRON International Corporation, Novato, CA, USA

1. INTRODUCTION

North American Background (NAB; formerly known as Policy Relevant Background or PRB) ozone concentrations have been defined by the U.S. Environmental Protection Agency as those that would occur in the absence of anthropogenic emissions in continental North America. In this context, NAB concentrations represent levels that are not controllable by regulations either in the U.S. or through agreements with neighboring North American countries. Processes that contribute to NAB ozone include natural sources globally and anthropogenic sources from outside of North America. Contributions to NAB ozone concentrations include photochemistry associated with natural emissions of volatile organic compounds (VOCs), oxides of nitrogen (NO_x), and carbon monoxide (CO) from biogenic emissions (not including agricultural activities), open fires, lightning, the long-range transport of ozone and its precursors from outside of North America, and stratospheric-tropospheric exchange (STE) of ozone (U.S. EPA 2013). NAB ozone concentrations, which are not directly measurable, are a construct of chemical transport models (Zhang et al. 2011; Emery et al. 2012; Henderson et al., 2012) that have been used to inform decisions about National Ambient Air Quality Standards (NAAQS) (McDonald-Buller et al., 2011). At the state-level, understanding the contributions of natural and transboundary anthropogenic sources can be important for effective air quality planning, especially under standards that may become increasingly stringent in the future. This work considered a state-level analysis of NAB ozone concentrations that

focused on Texas. A historical CAMx episode developed for regional air quality planning was used with boundary conditions from a high-resolution GEOS-Chem simulation. The objectives were to examine spatial gradients in surface NAB ozone across Texas, to compare NAB ozone on high versus low ozone days, and to investigate the vertical distribution in NAB ozone.

2. METHODS

2.1 Regional Modeling

A CAMx v 5.40 simulation for May 31-July 2, 2006 that was developed by the Texas Commission on Environmental Quality (TCEQ) to support air quality planning activities in the state (<http://www.tceq.texas.gov/airquality/airmod/rider8/rider8Modeling>) was used as the basis for the standard and NAB ozone simulations. Modifications were made to outer boundary conditions and to emissions inventories to include NO_x emissions for lightning and fire emissions estimates outside of Texas, in accordance with the objectives of examining NAB ozone sources. The horizontal grid domain is shown in Figure 1; the CAMx vertical grid spanned 28 layers from the surface to 13.6 km above ground level (AGL). Version 6 of the Carbon Bond mechanism (CB6) was employed for the gas-phase chemistry (Yarwood et al. 2010), and the Zhang model was used for dry deposition (Zhang et al., 2003). Meteorological data were developed using the Weather Research and Forecasting (WRF) ver. 3.1. Methane was set to 1750 ppbv. For the NAB ozone simulation in the North America region (10°N-70°N, 170°W-40°W), all anthropogenic emissions including those from ships, biofuels, aircraft NO_x, and fertilizer NO_x were removed.

*Corresponding author: Elena McDonald-Buller, Center for Energy and Environmental Resources, University of Texas at Austin, 10100 Burnet Rd, Building 133 Mail Code R7100; Austin, TX 78758; e-mail: ecmb@mail.utexas.edu

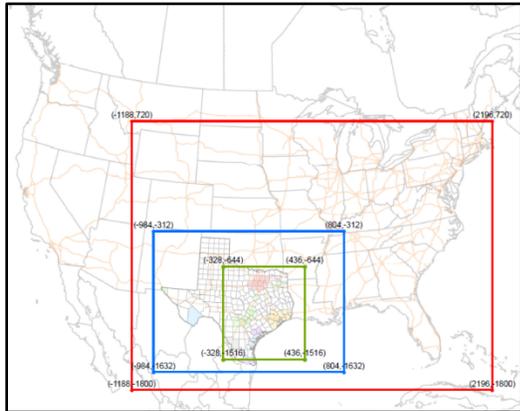


Fig. 1. Nested CAMx horizontal grid domains: 36-km U.S. (red), 12-km (blue) and 4-km (green).

2.2 GEOS-Chem Boundary Conditions

Boundary conditions for the U.S. 36-km grid were developed using GEOS-Chem v8-02-03. Zhang et al. (2011) describe the GEOS-Chem configuration and emissions inventories in detail. GEOS-Chem was run at $1/2^\circ \times 2/3^\circ$ horizontal resolution over North America for the standard and NAB ozone simulations. Boundary conditions for the nested North American simulation were provided by global GEOS-Chem simulations at $2^\circ \times 2.5^\circ$ horizontal resolution at a 3-h temporal resolution. Output fields of tracer concentrations, temperature, pressure at sea-level and vertical grid levels, and air density for the nested North American simulation at 3-h resolution were obtained for the CAMx period using the ND49 instantaneous 3-D time series diagnostic in GEOS-Chem. Morris et al. (2007) and Emery et al. (2012) describe the interface program used to interpolate GEOS-Chem concentration fields vertically and horizontally to obtain chemical boundary conditions for the 36-km CAMx domain and to map GEOS-Chem gas-phase species to Carbon Bond 5 (CB05). It was modified for this study to accommodate the finer horizontal resolution of the GEOS-Chem simulation over North America and mapping to CB6 species.

3. RESULTS

3.1 Measured MDA8 Ozone Concentrations

Time series of measured maximum daily 8-hour average (MDA8) ozone concentrations across four Texas urban areas, El Paso, Austin, Dallas/Fort Worth, and Houston-Galveston-Brazoria, during May 31-July 2 2006 are shown in

Figure 2. El Paso is located in far west Texas at the border with New Mexico and Chihuahua, Mexico, while the other three areas are located within the eastern half of the state. Houston-Galveston-Brazoria is located in southeast Texas on the Gulf of Mexico coastline. Austin is located in central Texas. Dallas-Fort Worth is located in northeastern Texas. Median MDA8 ozone concentrations in El Paso were approximately 60 ppb throughout the month of June. In contrast, high ozone days (defined here as ≥ 75 ppb) in eastern Texas occurred during two different large-scale weather regimes. June 3-15 had a primarily unvarying hot and dry weather pattern with high pressure dominant at the surface and upper levels. Periodic minor changes in upper level conditions resulted in the slow southward movement of weak cold fronts across portions of eastern Texas. These cold fronts were largely ill-defined in location and movement and represented diffuse transition zones separating relatively dry continental air to the north and moister maritime air to the south. Wind patterns in the lower atmosphere indicated regional stagnation. Measured high ozone during June 27-30 over eastern Texas followed the passage of a relatively strong cold front accompanied by a deep layer of northerly winds in the lower atmosphere that transported air into Texas from regions northward including the Central Plains region eastward to the Mississippi River Valley.

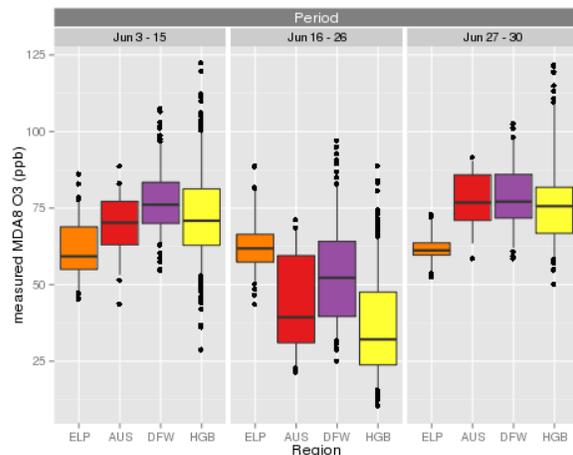


Fig.2 Measured MDA8 ozone concentrations averaged across the locations of monitors in El Paso (ELP), Austin (AUS), Dallas-Fort Worth (DFW) and Houston-Galveston-Brazoria (HGB) during June 2006. Boxes represent the second and third quartiles, whiskers represent the range of 5th to 95th percentile concentrations, and the dots represent outliers.

3.2 NAB Ozone at CASTNET Sites

Predicted NAB MDA8 ozone concentrations at CASTNET monitoring sites grouped by region (intermountain west, central, and east) in the U.S. domain are shown in Figure 3. Median NAB ozone concentrations in the intermountain west (30 ppbv) were greater than in the central and eastern U.S. (18 ppbv). Peak NAB MDA8 ozone concentrations were 44 ppbv in the intermountain west and 33 and 34 ppbv in the central and eastern U.S., respectively. These spatial patterns of NAB ozone concentrations were similar to those shown by Zhang et al. (2011) and Emery et al. (2012) that used different modeling configurations. NAB ozone concentrations during June 2006 (Figure 4a) between the two CASTNET sites in Texas reflected differences in altitude and geographic location. Median NAB MDA8 ozone concentrations were 17 ppbv at ALC188, Alabama-Coushatta, adjacent to the Houston-Galveston-Brazoria area, and 26 ppbv at BBE401 in Big Bend National Park in west Texas. Emery et al. (2012) found median NAB ozone values at Big Bend near 40 ppbv, similar to Zhang et al. (2011), over the summer and spring seasons of 2006.

3.3 NAB Ozone in Eastern Texas

Median NAB MDA8 ozone concentrations were 18-22 ppbv among most cities within eastern Texas. Maximum NAB MDA8 values were approximately 30 ppbv, but were as much as 41 ppbv in the Houston-Galveston-Brazoria area (Figure 4a). Little variability in median NAB MDA8 ozone concentrations was evident between days with observed high (≥ 75 ppbv; June 3-15 and June 27-30) and low ozone (June 16-26) concentrations (Figure 4b). In contrast, in El Paso, located within the intermountain west, the median NAB MDA8 ozone concentration was 29 ppbv with a peak value of 36 ppbv during June 16-26, with similar values during June 3-15. NAB MDA8 ozone concentrations were markedly lower, with median and maximum values of 20 ppbv and 23 ppbv, respectively, during June 27-30 in El Paso. The large-scale weather patterns suggested that eastern Texas and far west Texas were affected by different long-range transport patterns during the month. Transport of air from continental regions located to the north of eastern Texas occurred during June 3-15; in contrast, long-range transport patterns into El Paso originated from either the southeast (central Gulf of Mexico and northern Mexico) or southwest (Gulf of California and over northwest Mexico). During June 27-30,

both eastern Texas and west Texas were affected by long-range transport of air from continental regions located northward of the state.

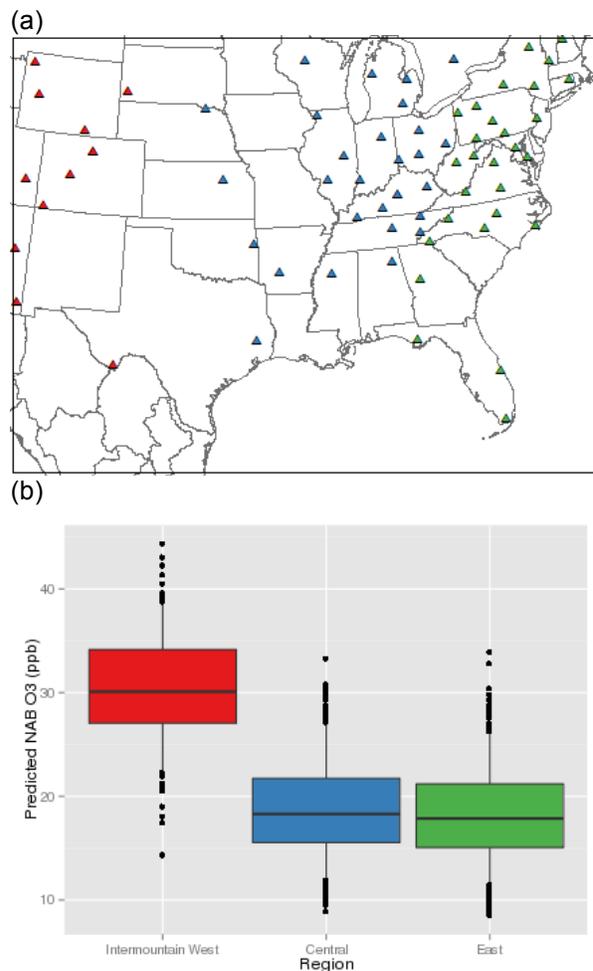


Fig. 3 (a) CASTNET sites grouped by region in the U.S. domain: intermountain west (red); central (blue), and east (green). (b) Predicted NAB MDA8 ozone concentration at CASTNET monitors in the intermountain west, central, and east regions of the U.S. domain. Boxes represent the second and third quartiles, whiskers represent the range of 5th to 95th percentile concentrations, and the dots represent outliers.

3.4 Vertical Distribution of Background Ozone

Modeled and observed hourly vertical ozone distributions were explored for specific days when ozonesonde launches occurred in Texas as part of the Tropospheric Ozone Pollution Project (Morris 2013). Model predictions from the standard simulations and sonde observations showed quite reasonable agreement in the magnitude and

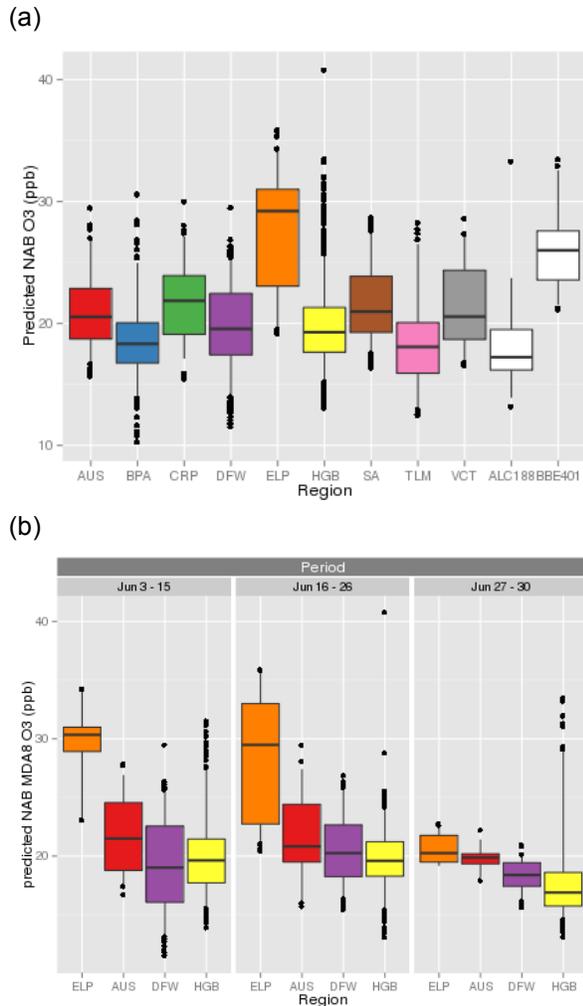


Fig. 4. (a) Predicted NAB MDA8 ozone concentrations for the locations of surface monitors during June 2006 in eastern Texas, El Paso, and two CASTNET sites (ref. Figure 1). (b) Predicted NAB MDA8 ozone concentrations in El Paso, Austin, Dallas-Fort Worth, and Houston-Galveston-Brazoria during June 3-15, June 16-26, and June 27-30, respectively. Boxes represent the second and third quartiles, whiskers represent the range of 5th to 95th percentile concentrations, and the dots represent outliers.

vertical distribution of ozone concentrations. Predicted NAB MDA8 ozone concentrations at the surface and within the vertical CAMx layers spanning 2.1-2.4 km and 4.9-5.8 km AGL are shown in Figure 5. Median NAB MDA8 ozone concentrations increased with altitude over Texas. While differences in NAB MDA8 concentrations between eastern Texas and far west Texas were pronounced at the surface, differences generally decreased with altitude. At the surface, median NAB MDA8 ozone concentrations in El Paso, at Big Bend National Park, and within the eastern

half of Texas were 29, 26, and 17-22 ppbv, respectively. At 2 km AGL, which approximated the height of the planetary boundary layer, NAB MDA8 ozone concentrations were 32-34 ppbv for all locations except Big Bend (39 ppbv). Vertical gradients in NAB ozone between the surface and 2 km AGL were less pronounced at the higher elevation locations of El Paso and Big Bend. At 5 km AGL, median NAB MDA8 ozone concentrations were 51-55 ppbv at all sites.

4. CONCLUSIONS

NAB ozone concentrations have historically been used to inform policy decisions about the federal air quality standard for ozone. At state- or regional-levels, understanding the contributions of natural sources and transboundary anthropogenic sources can be important for charting a path toward effective air quality management plans, in particular under standards that may become increasingly stringent in the future. This work demonstrated an analysis of NAB ozone concentrations at the state-level using a regional air quality model with a high-resolution global simulation. Texas has highly diverse climatology, land cover, and topography. Differences in NAB MDA8 ozone concentrations exist between urban ozone nonattainment and near nonattainment areas in eastern Texas and those located in the intermountain west. NAB ozone concentrations increased with altitude over Texas, with less pronounced gradients at higher elevation sites in west Texas. Related studies with different model configurations (Zhang et al., 2011; Emery et al. 2012; Zhang et al., 2013; Lin et al, 2012) and observational data (Kaynak et al., 2008; Jaffe and Wigder, 2012; Brodin et al., 2010; Jaffe et al., 2011) have indicated that elevation, arid climate, and natural sources such as lightning, wildfires, and stratospheric influence are factors that may contribute to elevated background ozone concentrations in the intermountain west. This work found that the variability in NAB MDA8 ozone concentrations during multi-day episodes with distinct transport patterns could differ from monthly or seasonal averages in Texas. This suggests the need for careful understanding of time periods selected for regulatory air quality modeling and planning efforts.

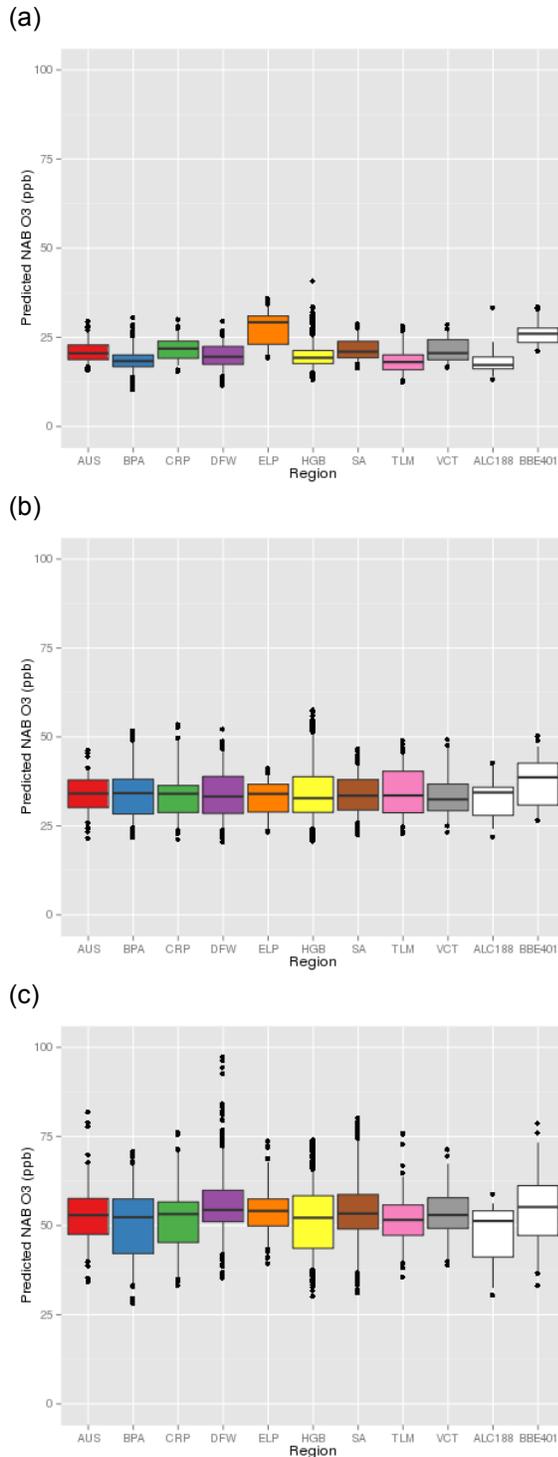


Fig. 5. Predicted NAB MDA8 ozone concentrations across the locations of monitors in eastern Texas urban areas, in El Paso, and at two Texas CASTNET sites at (a) the surface, (b) 2.1-2.4 km AGL, and (c) 4.9-5.8 km AGL during June 2006. Boxes represent the range of the second and third quartiles, whiskers represent the range of 5th to 95th percentile concentrations, and the dots represent outliers.

5. ACKNOWLEDGMENTS

This work was supported by a grant from the Texas Air Research Center (TARC) #312UTA0131A.

6. REFERENCES

Brodin, M., D. Helmig, and S. Oltmans, 2010: Seasonal ozone behavior along an elevation gradient in the Colorado Front Range Mountains. *Atmos. Environ.*, **44**, 5305-5315.

Emery, C., J. Jung, N. Downey, N., J. Johnson, M. Jimenez, G. Yarwood, and R. Morris, 2012: Regional and global modeling estimates of policy relevant background ozone over the United States. *Atmos. Environ.*, **47**, 206-217.

Henderson, B. H., N. Possiel, F. Akhtar, F., and H. Simon, 2012: Regional and seasonal analysis of North American background ozone from two studies, Memorandum to the Ozone NAAQS Review Docket EPA-HR-OAR-2012-0699.

Jaffe, D., 2011: Relationship between surface and free tropospheric ozone in the western US. *Environ. Sci. Technol.*, **25**, 432-438.

Jaffe D.A., and N. L. Wigder, 2012: Ozone production from wildfires: a critical review. *Atmos. Environ.*, **51**, 1-10.

Kaynak, B., Y. Hu, R.V. Martin, A.G Russell, Y. Choi, and Y. Wang, 2008: The effect of lightning NO_x production on surface ozone in the continental United States. *Atmos. Chem Phys.*, **8**, 5151-5159, doi:10.5194/acp-8-5151-2008.

Lin M., A. M. Fiore, O. R. Cooper, L.W. Horowitz, A. O. Langford, L. Hiram L., B. J. Johnson, V. Naik, S. Oltmans, and C. Senff, 2012: Springtime high surface ozone events over the western United States: Quantifying the role of stratospheric intrusions, *J. Geophys. Res.*, **117** D00V22, doi:10.1029/2012JD018151.

McDonald-Buller, E. C., D. T. Allen, N. Brown, D. J. Jacob, D. Jaffe, C. E. Kolb, A. S. Lefohn, S. Oltmans, D. Parrish, G. Yarwood, and L. Zhang, 2011: Establishing Policy Relevant Background (PRB) ozone concentrations in the United States. *Environ. Sci. Tech.*, **45**, 9484-9497.

Morris, R. E., B. Koo, B. Wang, G. Stella, D. McNally, C. Loomis, C.J. Chien, G. Tonnesen,

2007: Technical Support Document for VISTAS emissions and air quality modeling to support regional haze state implementation plans, Report to VISTAS Technical Coordinator. Available at: http://vistas-sesarm.org/documents/ENVIRON_Air_Quality_Modeling_Technical_Support_Document_11-14-07.pdf

Morris, G. A., 2013: Tropospheric Ozone Pollution Project, <http://physics.valpo.edu/ozone/index.html> (Accessed June 2013).

U.S. EPA, 2013: Integrated Science Assessment for Ozone and Related Photochemical Oxidants, EPA/600/R-10/076F, Office of Research and Development National Center for Environmental Assessment-RTP Division.

Yarwood G, J. Jung, G. Z. Whitten, G. Heo, J. Mellberg, and M. Estes, 2010: Updates to the Carbon Bond Mechanism for Version 6 (CB6). Presented at the 9th Annual CMAS Conference, Chapel Hill, October 2010.

Zhang L, D. J. Jacob, X. Yue, N. V. Downey, D. A. Wood, and D. Blewitt, 2013: Sources contributing to background surface ozone in the US Intermountain West *Atmos. Chem. Phys. Discuss.*, 13 25871-25909.

Zhang L., D. J. Jacob, N. V. Downey, D. A. Wood, D. Blewitt, C. C. Carouge, A van Donkelaar, D. B. A. Jones, L. T. Murray, and Y. Wang, 2011: Improved estimate of the policy-relevant background ozone in the United States using the GEOS-Chem global model with $1/2^\circ \times 2/3^\circ$ horizontal resolution over North America *Atmos. Environ.*, **45**, 6769-6776.

Zhang L, J. R. Brook, and R. Vet, 2003: A revised parameterization for gaseous dry deposition in air-quality models, *Atmos. Chem. Phys.*, **3**, 2067-2082.