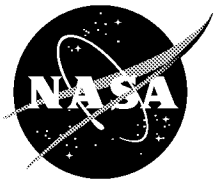
https://ntrs.nasa.gov/search.jsp?R=20010022512 2018-05-14T15:14:00+00:00Z

NASA/TM—2000–209891, Vol. 241



Technical Report Series on the Boreal Ecosystem-Atmosphere Study (BOREAS)

Forrest G. Hall and Sara K. Conrad, Editors

Volume 241

BOREAS TGB-10 Oxidant Concentration Data over the SSA

Hal Westberg and Brad Hall, Washington State University, Pullman
Andrea V. Jackson, Lancaster University, UK

National Aeronautics and
Space Administration

Goddard Space Flight Center
Greenbelt, Maryland 20771

November 2000

The NASA STI Program Office ... in Profile

Since its founding, NASA has been dedicated to the advancement of aeronautics and space science. The NASA Scientific and Technical Information (STI) Program Office plays a key part in helping NASA maintain this important role.

The NASA STI Program Office is operated by Langley Research Center, the lead center for NASA's scientific and technical information. The NASA STI Program Office provides access to the NASA STI Database, the largest collection of aeronautical and space science STI in the world. The Program Office is also NASA's institutional mechanism for disseminating the results of its research and development activities. These results are published by NASA in the NASA STI Report Series, which includes the following report types:

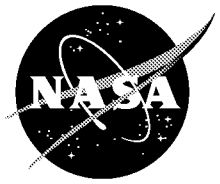
- TECHNICAL PUBLICATION. Reports of completed research or a major significant phase of research that present the results of NASA programs and include extensive data or theoretical analysis. Includes compilations of significant scientific and technical data and information deemed to be of continuing reference value. NASA's counterpart of peer-reviewed formal professional papers but has less stringent limitations on manuscript length and extent of graphic presentations.
- TECHNICAL MEMORANDUM. Scientific and technical findings that are preliminary or of specialized interest, e.g., quick release reports, working papers, and bibliographies that contain minimal annotation. Does not contain extensive analysis.
- CONTRACTOR REPORT. Scientific and technical findings by NASA-sponsored contractors and grantees.
- CONFERENCE PUBLICATION. Collected papers from scientific and technical conferences, symposia, seminars, or other meetings sponsored or cosponsored by NASA.
- SPECIAL PUBLICATION. Scientific, technical, or historical information from NASA programs, projects, and mission, often concerned with subjects having substantial public interest.
- TECHNICAL TRANSLATION. English-language translations of foreign scientific and technical material pertinent to NASA's mission.

Specialized services that complement the STI Program Office's diverse offerings include creating custom thesauri, building customized databases, organizing and publishing research results . . . even providing videos.

For more information about the NASA STI Program Office, see the following:

- Access the NASA STI Program Home Page at http://www.sti.nasa.gov/STI-homepage.html
- E-mail your question via the Internet to help@sti.nasa.gov
- Fax your question to the NASA Access Help Desk at (301) 621-0134
- Telephone the NASA Access Help Desk at (301) 621-0390
- Write to:
  NASA Access Help Desk
  NASA Center for AeroSpace Information
  7121 Standard Drive
  Hanover, MD 21076-1320

NASA/TM—2000–209891, Vol. 241



Technical Report Series on the Boreal Ecosystem-Atmosphere Study (BOREAS)

Forrest G. Hall and Sara K. Conrad, Editors

Volume 241

BOREAS TGB-10 Oxidant Concentration Data over the SSA

Hal Westberg and Brad Hall, Washington State University, Pullman
Andrea V. Jackson, Lancaster University, UK

National Aeronautics and
Space Administration

Goddard Space Flight Center
Greenbelt, Maryland 20771

November 2000

Available from:

NASA Center for AeroSpace Information
7121 Standard Drive
Hanover, MD 21076-1320
Price Code: A17

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Price Code: A10

BOREAS TGB-10 Oxidant Concentration Data over the SSA

Hal Westberg, Brad Hall, Andrea V. Jackson

Summary

The BOREAS TGB-10 team collected several trace gas data sets in its efforts to determine the role of biogenic hydrocarbon emissions with respect to boreal forest carbon cycles. This data set contains measured peroxide (H_2O_2 and total organic peroxides (ROOH)) and ozone concentrations as well as H_2O_2 and ROOH deposition velocities. These data were obtained at the SSA-OJP site from May to September 1994. The data are stored in tabular ASCII files.

Some important results were:

- Ozone concentrations were consistently low, 20-30 ppb, during the summer of 1994.
- Peroxide concentrations showed a seasonal variation with highest concentrations occurring in July (IFC-2).
- Midday H_2O_2 levels averaged around 1.4 ppb during IFC-2 and 0.4-0.5 ppb during IFC's 1 and 3.
- Midday organic peroxide concentrations were lower, averaging 0.8 ppb during IFC-2, and 0.4-0.5 ppb during IFC's 1 and 3.
- The rough pine forest canopy serves as a significant sink for H_2O_2.
- Midday H_2O_2 deposition velocities averaged 4-7 cm/s.
- Organic peroxide deposition velocities (measured as total ROOH) were approximately 40% as large as those of H_2O_2.

Table of Contents

1) Data Set Overview
2) Investigator(s)
3) Theory of Measurements
4) Equipment
5) Data Acquisition Methods
6) Observations
7) Data Description
8) Data Organization
9) Data Manipulations
10) Errors
11) Notes
12) Application of the Data Set
13) Future Modifications and Plans
14) Software
15) Data Access
16) Output Products and Availability
17) References
18) Glossary of Terms
19) List of Acronyms
20) Document Information

1. Data Set Overview

1.1 Data Set Identification

BOREAS TGB-10 Oxidant Concentration Data over the SSA

1.2 Data Set Introduction

The BOReal Ecosystem-Atmosphere Study (BOREAS) Trace Gas Biogeochemistry (TGB)-10 team collected oxidant concentration data at the Southern Study Area (SSA) Old Jack Pine (OJP) site during the growing season of 1994. Hydrogen peroxide was measured by the dual-channel, enzyme-catalyzed, fluorometric method using an instrument that was constructed at Washington State University (WSU). Ozone was measured with a Dasibi 1003-AH ozone sensor.

1.3 Objective/Purpose

Ambient concentrations of biogenic hydrocarbons, hydrogen peroxide, and organic hydroperoxides were determined. The data were used to examine (a) the role of biogenic hydrocarbon emissions with respect to carbon cycles in the boreal forest, (b) the chemical fate of boreal biogenic emissions, (c) the hypothesis that biospheric volatile organic carbon (VOC) emissions contribute to peroxide formation, and (d) the deposition rates of hydrogen peroxide and organic peroxides.

1.4 Summary of Parameters

The primary parameters are tropospheric concentrations of hydrogen peroxide and organic hydroperoxides in a boreal forest.

1.5 Discussion

None given.

1.6 Related Data Sets

BOREAS TGB-08 Monoterpene Concentration Data over the SSA
BOREAS TGB-08 Photosynthesis Data over the SSA
BOREAS TGB-08 Starch Data over the SSA
BOREAS TGB-09 Above Canopy Non-Methane Hydrocarbon Data over the SSA
BOREAS TGB-10 Oxidant Flux Data over the SSA
BOREAS TGB-10 Volatile Organic Carbon Data over the SSA

2. Investigator(s)

2.1 Investigator(s) Name and Title

Dr. Hal Westberg
Washington State University

Dr. Nick Hewitt
Lancaster University

2.2 Title of Investigation

Measurement of Biogenic Hydrocarbon Fluxes

2.3 Contact Information

Contact 1: Biogenic Hydrocarbon Emissions
Dr. Hal Westberg
Dept. of Civil and Environmental Engineering
Washington State University
Pullman, WA 99164-2710
(509) 335-1529
(509) 335-7632 (fax)
westberg@mail.wsu.edu

Contact 2: Deposition of Hydrogen Peroxide
Brad Hall
(Dr. Candis Claiborn)
Dept. of Civil and Environmental Engineering
Washington State University
Pullman, WA 99164-2710
(509) 335-5553
(509) 335-7632 (fax)
bhall@lar.ce.wsu.edu
claiborn@wsu.edu

Contact 3: Hydrogen Peroxide and Hydroperoxides
Andrea V. Jackson
(Dr. Nick Hewitt)
Environmental Science Division
Institute of Environmental and Biological Sciences
Lancaster University
Lancaster LA1 4QY
United Kingdom
(44-1524)-843854 (fax)
andrea@lec.leeds.ac.uk
n.hewitt@lancaster.ac.uk

Contact 4:
Jeffrey A. Newcomer
Raytheon ITSS
Code 923
NASA GSFC
Greenbelt, MD 20771
(301) 286-7858
(301) 286-0239 (fax)
Jeffrey.Newcomer@gsfc.nasa.gov

3. Theory of Measurements

Hydrogen peroxide and organic hydroperoxide measurements were determined by high performance liquid chromatography (HPLC) with fluorometric detection. Formaldehyde monitoring was performed by the reaction of formaldehyde with dinitrophenylhydrazine (DNPH).

4. Equipment

4.1 Sensor/Instrument Description

Hydrogen peroxide was measured by the dual-channel, enzyme-catalyzed, fluorometric method. The instrument was constructed at WSU, following the procedure outlined by K&K Instruments; Boulder, Colorado (Lazrus et al., 1986). Ozone was measured with a Dasibi 1003-AH ozone sensor.

4.1.1 Collection Environment

Tower-based measurements were conducted under ambient atmospheric conditions. Enclosure-based biogenic VOC measurements were conducted under near-ambient conditions, but at slightly elevated temperatures.

4.1.2 Source/Platform

All peroxide and ozone measurements were made from ground- or tower-mounted systems.

4.1.3 Source/Platform Mission Objectives

The objective of these experiments was to obtain canopy-scale fluxes of peroxides.

4.1.4 Key Variables

Ambient concentrations of the following trace gases were measured:

- isoprene
- alpha-pinene
- beta-pinene
- limonene
- monoterpenes
- hydrogen peroxide
- methylhydroperoxide
- hydroxymethlyhydroperoxide
- ozone

4.1.5 Principles of Operation

See Section 3.

4.1.6 Sensor/Instrument Measurement Geometry

Enclosure Sampling:

The instruments used for enclosure sampling were mounted on a battery-powered portable cart. The bag enclosure was mounted on a tripod base, allowing access to branches 1-3 meters from the ground.

Gradient Sampling:

Inlets were located on beams protruding 1 m off the west sides of the TF towers. With winds predominately from the south, west, or north, the samples usually contained unperturbed air. The inlet heights (above the forest floor) are summarized below.

```
OA    27.5 m and 37.5 m
OBS   12.4 m and 23.3 m
OJP   16.5 m and 23.8 m IFC-1, IFC-2
OJP   17.2 m and 23.8 m IFC-3
```

The lower inlet at the Old Jack Pine site was raised prior to IFC-3 to alleviate possible influences of the roughness sublayer.

4.1.7 Manufacturer of Sensor/Instrument

HP5890 gas chromatograph:
Hewlett Packard
15815 SE 37th St.
Bellevue, WA 98006

Dasibi 1003-AH ozone analyzer:
Dasibi Environmental
616 E. Colorado St.
Glendale, CA 91205

HP-3396A integrator:
Hewlett Packard
15815 SE 37th St.
Bellevue, WA 98006

The hydrogen peroxide system was custom-built at WSU:
WSU Technical Services
Washington State University
Pullman, WA 99164-2801

HPLC system:
Merck Ltd.
Merck House
Poole, Dorset
BH15 1TD, England

Data handling systems:
Labtech
400 Research Dr.
Wilmington, MA 01887

VG Data Systems
St. Georges Court
Hanover Business Park
Altrincham, Cheshire
WA14 5UG England

4.2 Calibration

Formaldehyde

High-purity formaldehyde-hydrazone was prepared by conventional methods for use as a master standard. The master standard was diluted to concentrations of 0.2, 0.5, 1.0, 2.0, and 5.0 ppm to establish calibration curves.

Sensors for the peripheral environmental measurements were calibrated at WSU prior to the field sampling program. Mass flow meters were tested against a precision wet-test meter at several flow rates. The thermocouples and amplifiers were calibrated against a National Institute for Standards and Technology (NIST) traceable mercury thermometer by measuring the response with all sensors immersed in a stirred ice-water bath slowly warmed to approximately 45 deg C. The humidity sensor was compared to calculated values for air passed through a temperature-controlled water bath. All of the sensor calibrations were performed using the PC laptop data system employed in the field.

Hydrogen Peroxide

The continuous hydroperoxide system was calibrated twice daily with liquid standards of hydrogen peroxide in deionized water. The standards were prepared at the 10-8 M level by serial dilution of a 30% H_2O_2 reagent (Fisher). The concentration of the primary reagent was determined by titration against KMnO4, which was then titrated against a NIST-traceable sodium oxalate solution.

Line losses through the PFA Teflon tubing were measured before and after each IFC. A gas-phase H_2O_2 generation system was used to produce a sample stream with near-ambient levels of H_2O_2. Line losses were determined by sampling this stream with and without the tower sampling line. A critical aspect of the peroxide gradient system is the potential for bias introduced in the two separate inlet sections. Care was taken to ensure that bias introduced by the valve and 4-m inlet sections was well-known and correctable. Relative bias was determined every few days by placing both inlets at the same height and sampling ambient air for several hours. Subsequent gradients were corrected for bias, which ranged from -1 to 9%. When the bias surpassed 7%, samples were rejected and the valve and sample lines were cleaned with methanol, deionized water, and peroxide-free air. After cleaning, bias was reduced to a nondetectable level.

Hydroperoxides

Peak identities were confirmed by comparison with retention times of authentic standards. Quantification was based on system response to hydrogen peroxide, as the same fluorescent dimer is formed for all hydroperoxides. Calibration was carried out twice daily and was found to be linear over the range $8x10^{-8}$ M to $5x10^{-6}$ M. The limit of detection has been determined to be less than 50 pptv.

Ozone

The Dasibi ozone monitor was calibrated against a Dasibi ozone source/monitor model 1008-PC (serial #3226).

4.2.1 Specifications

Hydrogen Peroxide

The H_2O_2 gradient measurements were occasionally subject to bias. It was extremely difficult to maintain clean sampling conditions at all times. Inlet filters cannot be used due to the potential for severe H_2O_2 loss on filter surfaces. Periods of unacceptable bias were encountered during the first IFC when the jack pine trees were pollinating, and occasionally during IFC-2 and IFC-3 when bugs would collect in the sample lines. The sample lines were sequentially flushed with methanol, water, and dry air periodically to remove dirt, pollen, and bugs.

Ozone

The source instrument was recently compared to other instruments at the University of Idaho, and was found to agree within 1-2 ppb.

4.2.1.1 Tolerance

None given.

4.2.2 Frequency of Calibration

Calibrations were performed before and after each IFC. Bias checks for peroxide gradients were performed every few days during IFC-2 and IFC-3. No bias checks were performed during IFC-1.

4.2.3 Other Calibration Information

None given.

5. Data Acquisition Methods

Hydrogen Peroxide and Organic Hydroperoxide

Measurements Air was drawn at 4 L/min from the inlet (24 m height) on the TF tower through 1/4" TFE Teflon tubing to the tower base, where a gas-phase scrubber was used to scrub peroxides from the air stream. Samples were collected in 5 mL deionized water. HPLC analysis was performed immediately after sample collection.

HPLC separation was achieved on a Absorbosphere MF Plus C18 column (Altech) with an eluent of 0.001 M sulfuric acid with 0.0001 M EDTA delivered by a Merck-Hitachi L-6200 Intelligent HPLC pump at a flow rate of 0.6 mL/min. After separation, the peroxides were derivatized by addition of 0.026 M p-hydroxyphenylacetic acid with 10,000 units/L of horseradish peroxidase (type II Sigmal Chemical) in 0.5 M potassium hydrogen phthalate buffer at pH 5.8. The reaction of the fluorescence reagent with the separated hydroperoxides takes place in a Teflon coil to ensure adequate mixing. Following this, the pH of the resulting solution is raised to above 10 to convert the dimer to its fluorescent anionic form using a membrane reactor constructed of Nafion (DuPont) tubing immersed in 30% ammonium hydroxide solution. Fluorescence measurements were made using a Merck-Hitachi spectrophotometer with excitation and emission wavelengths of 310 and 405 nm, respectively. The HPLC analytical system was located in the instrument hut.

Formaldehyde Monitoring

A DNPH/silica cartridge was connected to the inlet end of a 1/4" stainless steel tube extending to 3 m above the ground. The sample flow (1 L/min) was generated with a small pump and monitored with a Matheson flow meter. A calibrated Tylan digital totalizer was used to record the total volume sampled. The cartridges were exposed to the ambient air for nominal durations of 2, 4, or 6 hours. Cartridges were brought back to WSU for analysis.

Sample and blank cartridges were eluted with 3 mL acetonitrile. Hydrazone concentrations in the eluent were determined by reverse-phase HPLC. The HPLC analysis was performed using an LKB modular system consisting of two pumps (LKB #2150), a 190-600 nm ultraviolet/visible wavelength detector (LKB #2151) operated at 360 nm, and an LC gradient controller (LKB # 2152). A Brownlee-Rainin 10-cm OD-MPS column (or comparable) with a hydrophobic, nonpolar stationary phase (bonded on 5-micrometer spheres), preceded by a similar guard column was used for peak separation. A gradient elution, beginning with a 50:50 water:acetonitrile ratio was used, changing to a 30:70 water:acetonitrile ratio over a period of 21 minutes. The column flow rate was 0.5 mL/min, and the sample loop volume was 20 microliters.

Signals from the hydrogen peroxide and ozone instruments (TGB-10b) were stored as 1-minute averages via PC. Data acquisition software from Labtech was used to record signals (voltages). The gas chromatograph was interfaced to a pair of HP-3396A integrators for peak integration. Raw signals were also stored via PC for data reprocessing. The HPLC system for hydroperoxides was interfaced with a VG Data Systems Minichrom data acquisition system for chromatography. The connection of the HPLC to the data system was achieved using a chromatography server.

6. Observations

6.1 Data Notes

Hydrogen Peroxide

Periods of unacceptable bias were encountered during the first IFC, when the jack pine trees were pollinating, and occasionally during IFC-2 and IFC-3, when bugs would collect in the sample lines.

Ozone

Some problems with the electronic zero were detected during IFC-1. An offset of -6 ppb relative to the data acquisition system was discovered. This offset was easily measured on a daily basis, and remained essentially unchanged throughout the experiment.

6.2 Field Notes

TGB-10 peroxide data were deemed questionable (QC = 2) or unacceptable (QC = 3) during the following periods:

```
C *** QUALITY CONTROL (based local TIME and DAY)

25-May-1994          QC = 2          poor calibration
26-May-1994          QC = 2          poor calibration
27-May-1994          QC = 2          poor calibration
04-Jul-1994          QC = 3          extreme pollen event
05-Jul-1994          QC = 3          extreme pollen event
06-Jul-1994          QC = 2          moderate pollen event
09-Jul-1995          QC = 2          bias unknown
25-Jul-1994          QC = 2          poor calibration
31-Jul-1994          QC = 3          high noise level
04-Aug-1994          QC = 2          smoke
05-Aug-1994          QC = 2          smoke
06-Aug-1994          QC = 3          rain
01-Sep-1994          QC = 2          lost signal
02-Sep-1994          QC = 3          suspect line loss
```

7. Data Description

7.1 Spatial Characteristics

7.1.1 Spatial Coverage

Peroxide and ozone concentrations were measured near the OJP tower flux site only. The North American Datum of 1983 (NAD83) coordinates for the site are:

```
SSA-OJP:  53.91634N, 104.69203W
```

7.1.2 Spatial Coverage Map

Not available.

7.1.3 Spatial Resolution

The data are point source measurements at the given locations.

7.1.4 Projection

Not applicable.

7.1.5 Grid Description

Not applicable.

7.2 Temporal Characteristics

7.2.1 Temporal Coverage

Measurements were taken at SSA-OJP from 25-May-1994 to 09-Sep-1994.

7.2.2 Temporal Coverage Map

Not available.

7.2.3 Temporal Resolution

Peroxide and ozone concentrations were measured continuously during daylight hours. In addition, many overnight sampling periods were obtained. No regular intervals of data collection were done at the site; however, data were collected on several days during the growing season of 1994.

7.3 Data Characteristics

7.3.1 Parameter/Variable

The parameters contained in the data files on the CD-ROM are:

Column Name
SITE_NAME
SUB_SITE
DATE_OBS
TIME_OBS
SAMPLE_SIZE
HT_AGL
MEAN_H2O2_CONC
SDEV_H2O2_CONC
MEAN_ROOH_CONC
SDEV_ROOH_CONC
MEAN_O3_CONC
SDEV_O3_CONC
QUALITY_CODE
CRTFCN_CODE
REVISION_DATE

7.3.2 Variable Description/Definition

The descriptions of the parameters contained in the data files on the CD-ROM are:

Column Name	Description
SITE_NAME	The identifier assigned to the site by BOREAS, in the format SSS-TTT-CCCCC, where SSS identifies the portion of the study area: NSA, SSA, REG, TRN, and TTT identifies the cover type for the site, 999 if unknown, and CCCCC is the identifier for site, exactly what it means will vary with site type.
SUB_SITE	The identifier assigned to the sub-site by BOREAS, in the format GGGGG-IIIII, where GGGGG is the group associated with the sub-site instrument, e.g. HYD06 or STAFF, and IIIII is the identifier for sub-site, often this will refer to an instrument.
DATE_OBS	The date on which the data were collected.
TIME_OBS	The Greenwich Mean Time (GMT) when the data were collected.
SAMPLE_SIZE	The number of one minute sampling periods that were used to compute the average concentration (data were stored as 1 min averages of the continuous signal).
HT_AGL	The height above ground at which the measurements were taken.
MEAN_H2O2_CONC	The mean hydrogen peroxide concentration.

SDEV_H2O2_CONC	Standard deviation of the peroxide concentration
MEAN_ROOH_CONC	The mean organic peroxide concentration.
SDEV_ROOH_CONC	Standard deviation of the organic peroxide concentration.
MEAN_O3_CONC	The mean ozone concentration.
SDEV_O3_CONC	The standard deviation of the ozone concentration.
QUALITY_CODE	1:good data: normal operation, 2:good data: normal operation, but uncertainties are greater due to non-ideal sampling condition or equipment function, 3:data questionable or possible instrument malfunction
CRTFCN_CODE	The BOREAS certification level of the data. Examples are CPI (Checked by PI), CGR (Certified by Group), PRE (Preliminary), and CPI-??? (CPI but questionable).
REVISION_DATE	The most recent date when the information in the referenced data base table record was revised.

7.3.3 Unit of Measurement

The measurement units for the parameters contained in the data files on the CD-ROM are:

Column Name	Units
SITE_NAME	[none]
SUB_SITE	[none]
DATE_OBS	[DD-MON-YY]
TIME_OBS	[HHMM GMT]
SAMPLE_SIZE	[unitless]
HT_AGL	[meters]
MEAN_H2O2_CONC	[parts per billion]
SDEV_H2O2_CONC	[parts per billion]
MEAN_ROOH_CONC	[parts per billion]
SDEV_ROOH_CONC	[parts per billion]
MEAN_O3_CONC	[nanomoles O3][mole air^-1]
SDEV_O3_CONC	[nanomoles O3][mole air^-1]
QUALITY_CODE	[unitless]
CRTFCN_CODE	[none]
REVISION_DATE	[DD-MON-YY]

7.3.4 Data Source

The sources of the parameter values contained in the data files on the CD-ROM are:

Column Name	Data Source
SITE_NAME	Not applicable
SUB_SITE	Not applicable
DATE_OBS	Investigator
TIME_OBS	Investigator
SAMPLE_SIZE	Investigator
HT_AGL	Investigator
MEAN_H2O2_CONC	Gas Chromatograph, HPLC
SDEV_H2O2_CONC	Gas Chromatograph, HPLC]
MEAN_ROOH_CONC	Gas Chromatograph, HPLC
SDEV_ROOH_CONC	Gas Chromatograph, HPLC
MEAN_O3_CONC	Gas Chromatograph, HPLC

SDEV_O3_CONC	Gas Chromatograph, HPLC
QUALITY_CODE	Investigator
CRTFCN_CODE	Not applicable
REVISION_DATE	Not applicable

7.3.5 Data Range

The following table gives information about the parameter values found in the data files on the CD-ROM.

Column Name	Minimum Data Value	Maximum Data Value	Missng Data Value	Unrel Data Value	Below Detect Limit	Data Not Cllctd
SITE_NAME	SSA-OJP-FLXTR	SSA-OJP-FLXTR	None	None	None	None
SUB_SITE	TGB10-CON01	TGB10-CON01	None	None	None	None
DATE_OBS	25-MAY-94	09-SEP-94	None	None	None	None
TIME_OBS	0	2358	None	None	None	None
SAMPLE_SIZE	0	43	None	None	None	None
HT_AGL	3	23	None	None	None	None
MEAN_H2O2_CONC	.03	4.21	-999	None	None	None
SDEV_H2O2_CONC	0	.47	-999	None	None	None
MEAN_ROOH_CONC	0	1.57	-999	None	None	None
SDEV_ROOH_CONC	0	.35	-999	None	None	None
MEAN_O3_CONC	2	27.6	-999	None	None	None
SDEV_O3_CONC	0	20.7	-999	None	None	None
QUALITY_CODE	1	3	None	None	None	None
CRTFCN_CODE	CPI	CPI	None	None	None	None
REVISION_DATE	24-OCT-96	24-OCT-96	None	None	None	None

Minimum Data Value -- The minimum value found in the column.
Maximum Data Value -- The maximum value found in the column.
Missng Data Value -- The value that indicates missing data. This is used to indicate that an attempt was made to determine the parameter value, but the attempt was unsuccessful.
Unrel Data Value -- The value that indicates unreliable data. This is used to indicate an attempt was made to determine the parameter value, but the value was deemed to be unreliable by the analysis personnel.
Below Detect Limit -- The value that indicates parameter values below the instruments detection limits. This is used to indicate that an attempt was made to determine the parameter value, but the analysis personnel determined that the parameter value was below the detection limit of the instrumentation.
Data Not Cllctd -- This value indicates that no attempt was made to determine the parameter value. This usually indicates that BORIS combined several similar but not identical data sets into the same data base table but this particular science team did not measure that parameter.

Blank -- Indicates that blank spaces are used to denote that type of value.
N/A -- Indicates that the value is not applicable to the respective column.
None -- Indicates that no values of that sort were found in the column.

7.4 Sample Data Record

The following are wrapped versions of data record from a sample data file on the CD-ROM.

```
SITE_NAME,SUB_SITE,DATE_OBS,TIME_OBS,SAMPLE_SIZE,HT_AGL,MEAN_H2O2_CONC,
SDEV_H2O2_CONC,MEAN_ROOH_CONC,SDEV_ROOH_CONC,MEAN_O3_CONC,SDEV_O3_CONC,
QUALITY_CODE,CRTFCN_CODE,REVISION_DATE
'SSA-OJP-FLXTR','TGB10-CON01',25-MAY-94,546,9,17.0,.56,.02,.39,.01,-999.0,
-999.0,2,'CPI',24-OCT-96
'SSA-OJP-FLXTR','TGB10-CON01',25-MAY-94,611,15,23.0,.64,.05,.42,.02,-999.0,
-999.0,2,'CPI',24-OCT-96
'SSA-OJP-FLXTR','TGB10-CON01',25-MAY-94,630,15,17.0,.51,.04,.45,.02,-999.0,
-999.0,2,'CPI',24-OCT-96
'SSA-OJP-FLXTR','TGB10-CON01',25-MAY-94,650,16,23.0,.61,.04,.42,.01,-999.0,
-999.0,2,'CPI',24-OCT-96
```

8. Data Organization

8.1 Data Granularity

The smallest unit of data tracked by the BOREAS Information System (BORIS) was the data measured on a particular date at a particular site.

8.2 Data Format(s)

The Compact Disk-Read-Only Memory (CD-ROM) files contain American Standard Code for Information Interchange (ASCII) numerical and character fields of varying length separated by commas. The character fields are enclosed with single apostrophe marks. There are no spaces between the fields.

Each data file on the CD-ROM has four header lines of Hyper-Text Markup Language (HTML) code at the top. When viewed with a Web browser, this code displays header information (data set title, location, date, acknowledgments, etc.) and a series of HTML links to associated data files and related data sets. Line 5 of each data file is a list of the column names, and line 6 and following lines contain the actual data.

9. Data Manipulations

9.1 Formulae

The peroxide gradient was computed from three successive measurements of peroxide concentration at two levels (10-18 minutes at each level).

Peroxide_gradient = (C2 - 0.5*(C1+C3))/delta_Z

where: C1 = concentration measured at lower level (period t)
C2 = concentration measured at upper level (period t+1)
C3 = concentration measured at lower level (period t+2)

Special note: If the standard error associated with C1,C2,or C3 was greater than 0.05%,the peroxide gradient was deemed unacceptable. This procedure was performed in order to screen periods of highly variable concentration, which might suggest unsteady-state conditions (gusts or large eddies), which are not conducive to K-theory. This data screening procedure helps eliminate many unrealistic deposition velocities, but does not affect the overall conclusions.

Peroxide_deposition_velocity = (peroxide_gradient)/(C_avg)*(eddy_diffusivity)

where: C_avg = average peroxide concentration (over both levels)

9.1.1 Derivation Techniques and Algorithms
None given.

9.2 Data Processing Sequence

9.2.1 Processing Steps
BORIS staff processed the data by:
- Reviewing the initial data files and loading them online for BOREAS team access.
- Designing relational data base tables to inventory and store the data.
- Loading the data into the relational data base tables.
- Performing the conversions on measurements into System International (SI) units.
- Extracting the standardized data into logical files.

9.2.2 Processing Changes
None.

9.3 Calculations
None.

9.3.1 Special Corrections/Adjustments

Peroxide Bias adjustment: C1 = C1*fb C3 = C1*fb

where: fb = bias relative to upper sampling level
(range 0.99 to 1.07 for H_2O_2, 0.99 to 1.02 for ROOH)

9.3.2 Calculated Variables
None given.

9.4 Graphs and Plots
None.

10 Errors

10.1 Sources of Error
Hydrogen Peroxide: The following sources of error are those that are not easily identified, and may affect the data record despite efforts to identify and correct all errors:
- Irregularities in sample line loss (condensation, dirt, bugs).
- Contamination of the switching valve due to bugs, dirt, pollen, etc.
- Irregular signal drift, possibly due to extreme temperature fluctuations.
- Interference due to smoke particles.

Hydroperoxides:
- Fluctuations in air flow rate.
- Error in preparing sample volume.
- Fluctuations in sample collection efficiency with temperature.
- Possible condensation in sample lines.
- Interference due to smoke particles.
- Error associated with the serial dilution of H_2O_2 standards.

10.2 Quality Assessment

10.2.1 Data Validation by Source
None given.

10.2.2 Confidence Level/Accuracy Judgment
Hydrogen peroxide concentrations are good to approximately 30%. Total organic peroxide concentrations have not been corrected for collection efficiency. Reported total organic peroxide concentration may be underestimated by as much as 60%. Individual deposition velocity measurements are subject to 50-80% uncertainty due to uncertainties in the measured gradient, the measured eddy diffusivity, and the natural variability of a turbulent atmosphere. Ozone concentrations are good to +/- 5 ppb for IFC-1, and +/- 3 ppb for IFC-2 and IFC-3.

10.2.3 Measurement Error for Parameters
None given.

10.2.4 Additional Quality Assessments
None.

10.2.5 Data Verification by Data Center
Data were examined for general consistency and clarity.

11. Notes

11.1 Limitations of the Data
None given.

11.2 Known Problems with the Data
None given.

11.3 Usage Guidance
None given.

11.4 Other Relevant Information
None given.

12. Application of the Data Set

The data can be used to examine (a) the role of biogenic hydrocarbon emissions with respect to carbon cycles in the boreal forest, (b) the chemical fate of boreal biogenic emissions, (c) the hypothesis that biospheric volatile organic carbon (VOC) emissions contribute to peroxide formation, and (d) the deposition rates of hydrogen peroxide and organic peroxides.

13. Future Modifications and Plans

None.

14. Software

14.1 Software Description

All software programs used to gather data were off-the-shelf, standard scientific packages.

14.2 Software Access

None given.

15. Data Access

The TGB-10 oxidant concentration data are available from the Earth Observing System Data and Information System (EOSDIS) Oak Ridge National Laboratory (ORNL) Distributed Active Archive Center (DAAC).

15.1 Contact Information

For BOREAS data and documentation please contact:

ORNL DAAC User Services
Oak Ridge National Laboratory
P.O. Box 2008 MS-6407
Oak Ridge, TN 37831-6407
Phone: (423) 241-3952
Fax: (423) 574-4665
E-mail: ornldaac@ornl.gov or ornl@eos.nasa.gov

15.2 Data Center Identification

Earth Observing System Data and Information System (EOSDIS) Oak Ridge National Laboratory (ORNL) Distributed Active Archive Center (DAAC) for Biogeochemical Dynamics http://www-eosdis.ornl.gov/.

15.3 Procedures for Obtaining Data

Users may obtain data directly through the ORNL DAAC online search and order system [http://www-eosdis.ornl.gov/] and the anonymous FTP site [ftp://www-eosdis.ornl.gov/data/] or by contacting User Services by electronic mail, telephone, fax, letter, or personal visit using the contact information in Section 15.1.

15.4 Data Center Status/Plans

The ORNL DAAC is the primary source for BOREAS field measurement, image, GIS, and hardcopy data products. The BOREAS CD-ROM and data referenced or listed in inventories on the CD-ROM are available from the ORNL DAAC.

16. Output Products and Availability

16.1 Tape Products

None.

16.2 Film Products

None.

16.3 Other Products

These data are available on the BOREAS CD-ROM series.

17. References

17.1 Platform/Sensor/Instrument/Data Processing Documentation

None given.

17.2 Journal Articles and Study Reports

Guenther, A. et al. 1996. Isoprene fluxes measured by enclosure, relaxed eddy accumulation, surface layer gradient, mixed layer gradient, and mixed layer mass balance techniques. Journal of Geophysical Research, 101, 18,555-18,567.

Hall, B.D. and C.S. Claiborn. 1997. Measurements of the dry deposition of peroxides to a Canadian boreal forest. Journal of Geophysical Research 102(D24):29,343-29,353.

Lazrus, A.L, G.L. Kok, S.N. Gitlin, J.A. Lind, B.G. Heikes, and R.E. Shetter. 1986. Automated fluorometric method for hydrogen peroxide in air. Anal. Chem. 58, 594-597.

Kok, G.L., S.E. McLaren, and T.A. Staffelbach. 1995. HPLC determination of atmospheric organic hydroperoxides. J. Atmos. Ocean Tech., 12, 282-289.

Newcomer, J., D. Landis, S. Conrad, S. Curd, K. Huemmrich, D. Knapp, A. Morrell, J. Nickeson, A. Papagno, D. Rinker, R. Strub, T. Twine, F. Hall, and P. Sellers, eds. 2000. Collected Data of The Boreal Ecosystem-Atmosphere Study. NASA. CD-ROM.

Sellers, P. and F. Hall. 1994. Boreal Ecosystem-Atmosphere Study: Experiment Plan. Version 1994-3.0, NASA BOREAS Report (EXPLAN 94).

Sellers, P. and F. Hall. 1996. Boreal Ecosystem-Atmosphere Study: Experiment Plan. Version 1996-2.0, NASA BOREAS Report (EXPLAN 96).

Sellers, P., F. Hall, and K.F. Huemmrich. 1996. Boreal Ecosystem-Atmosphere Study: 1994 Operations. NASA BOREAS Report (OPS DOC 94).

Sellers, P., F. Hall, and K.F. Huemmrich. 1997. Boreal Ecosystem-Atmosphere Study: 1996 Operations. NASA BOREAS Report (OPS DOC 96).

Sellers, P., F. Hall, H. Margolis, B. Kelly, D. Baldocchi, G. den Hartog, J. Cihlar, M.G. Ryan, B. Goodison, P. Crill, K.J. Ranson, D. Lettenmaier, and D.E. Wickland. 1995. The boreal ecosystem-atmosphere study (BOREAS): an overview and early results from the 1994 field year. Bulletin of the American Meteorological Society. 76(9):1549-1577.

Sellers, P.J., F.G. Hall, R.D. Kelly, A. Black, D. Baldocchi, J. Berry, M. Ryan, K.J. Ranson, P.M. Crill, D.P. Lettenmaier, H. Margolis, J. Cihlar, J. Newcomer, D. Fitzjarrald, P.G. Jarvis, S.T. Gower, D. Halliwell, D. Williams, B. Goodison, D.E. Wickland, and F.E. Guertin. 1997. BOREAS in 1997: Experiment Overview, Scientific Results and Future Directions. Journal of Geophysical Research 102(D24): 28,731-28,770.

17.3 Archive/DBMS Usage Documentation

None.

18. Glossary of Terms

None.

19. List of Acronyms

```
ASCII   - American Standard Code for Information Interchange
BOREAS  - BOReal Ecosystem-Atmosphere Study
BORIS   - BOREAS Information System
CD-ROM  - Compact Disk-Read-Only Memory
DAAC    - Distributed Active Archive Center
DNPH    - dinitrophenylhydrazine
EOS     - Earth Observing System
EOSDIS  - EOS Data and Information System
GIS     - Geographic Information System
GMT     - Greenwich Mean Time
GSFC    - Goddard Space Flight Center
HPLC    - High Performance Liquid Chromatography
HTML    - Hyper-Text Markup Language
IFC     - Intensive Field Campaign
NAD83   - North American Datum of 1983
NASA    - National Aeronautics and Space Administration
NIST    - National Institute for Standards and Technology
NMHC    - Non-Methane Hydrocarbon
NSA     - Northern Study Area
OA      - Old Aspen
OBS     - Old Black Spruce
OJP     - Old Jack Pine
ORNL    - Oak Ridge National Laboratory
PANP    - Prince Albert National Park
REA     - Relaxed Eddy Accumulation
SI      - System International
SSA     - Southern Study Area
TF      - Tower Flux
TGB     - Trace Gas Biogeochemistry
URL     - Uniform Resource Locator
VOC     - Volatile Organic Compound (or Carbon)
WSU     - Washington State University
```

20. Document Information

20.1 Document Revision Dates

Written: 17-Nov-1994
Last Updated: 16-Jul-1999

20.2 Document Review Dates

BORIS Review: 12-Jun-1998
Science Review:

20.3 Document ID

20.4 Citation

When using these data, please contact the personnel listed in Section 2.3 and cite any relevant papers in Section 17.2:

If using data from the BOREAS CD-ROM series, also reference the data as:

Westberg , H. and N. Hewitt, "Measurement of Biogenic Hydrocarbon Fluxes." In Collected Data of The Boreal Ecosystem-Atmosphere Study. Eds. J. Newcomer, D. Landis, S. Conrad, S. Curd, K. Huemmrich, D. Knapp, A. Morrell, J. Nickeson, A. Papagno, D. Rinker, R. Strub, T. Twine, F. Hall, and P. Sellers. CD-ROM. NASA, 2000.

Also, cite the BOREAS CD-ROM set as:

Newcomer, J., D. Landis, S. Conrad, S. Curd, K. Huemmrich, D. Knapp, A. Morrell, J. Nickeson, A. Papagno, D. Rinker, R. Strub, T. Twine, F. Hall, and P. Sellers, eds. Collected Data of The Boreal Ecosystem-Atmosphere Study. NASA. CD-ROM. NASA, 2000.

20.5 Document Curator

20.6 Document URL

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	November 2000	Technical Memorandum

4. TITLE AND SUBTITLE
Technical Report Series on the Boreal Ecosystem-Atmosphere Study (BOREAS)
BOREAS TGB-10 Oxidant Concentration Data over the SSA

5. FUNDING NUMBERS
923
RTOP: 923-462-33-01

6. AUTHOR(S)
Hal Westberg, Brad Hall, and Andrea V. Jackson
Forrest G. Hall and Sara K. Conrad, Editors

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS (ES)
Goddard Space Flight Center
Greenbelt, Maryland 20771

8. PEFORMING ORGANIZATION REPORT NUMBER
2000-03136-0

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS (ES)
National Aeronautics and Space Administration
Washington, DC 20546-0001

10. SPONSORING / MONITORING AGENCY REPORT NUMBER
TM—2000–209891
Vol. 241

11. SUPPLEMENTARY NOTES
H. Westberg and B. Hall: Washington State University, Pullman; A.V. Jackson: Lancaster University, UK; S.K. Conrad: Raytheon ITSS

12a. DISTRIBUTION / AVAILABILITY STATEMENT
Unclassified–Unlimited
Subject Category: 43
Report available from the NASA Center for AeroSpace Information,
7121 Standard Drive, Hanover, MD 21076-1320. (301) 621-0390.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

The BOREAS TGB-10 team collected several trace gas data sets in its efforts to determine the role of biogenic hydrocarbon emissions with respect to boreal forest carbon cycles. This data set contains measured peroxide (H_2O_2 and total organic peroxides (ROOH)) and ozone concentrations as well as H_2O_2 and ROOH deposition velocities. These data were obtained at the SSA-OJP site from May to September 1994. The data are stored in tabular ASCII files. Some important results were:

- Ozone concentrations were consistently low, 20-30 ppb, during the summer of 1994.
- Peroxide concentrations showed a seasonal variation with highest concentrations occurring in July (IFC-2).
- Midday H_2O_2 levels averaged around 1.4 ppb during IFC-2 and 0.4-0.5 ppb during IFC's 1 and 3.
- Midday organic peroxide concentrations were lower, averaging 0.8 ppb during IFC-2, and 0.4-0.5 ppb during IFC's 1 and 3.
- The rough pine forest canopy serves as a significant sink for H_2O_2.
- Midday H_2O_2 deposition velocities averaged 4-7 cm/s.
- Organic peroxide deposition velocities (measured as total ROOH) were approximately 40% as large as those of H_2O_2.

14. SUBJECT TERMS
BOREAS, trace gas biogeochemistry.

15. NUMBER OF PAGES
18

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	UL