Atmospheric Sciences

Exponent®

CALNO2
Users Guide

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Introduction

CALNO2 is a post-processor for the CALPUFF system which has been developed to allow calculations of NO_2 concentrations based on modeled NO_x. The post-processor is run after the completion of CALPUFF simulations and will calculate NO_2 based on modeled NO_x using one of two methods: 1) the Ambient Ratio Method (ARM) or 2) the Ozone Limiting Method (OLM). The application of both methods has been implemented in coordination with the British Columbia Ministry of Environment and Climate Change Strategy (BCMOE) and is consistent with Guidance contained in the *Guidance for NO_2 Dispersion Modeling in British Columbia* (BCENV 2021).

After CALNO2 has been run, the output concentrations will be stored in a new CALPUFF format concentration file where the NO_x species has been replaced with NO_2. Further processing of this file can then be completed using other available CALPUFF post-processors including CALSUM, POSTUTIL and CALPOST.

The following sections provide details on the methods and requirements for running CALNO2. The sections are organized to follow through individual sections of the CALNO2 input control file and explain the variables and files required. A full copy of an example CALNO2 input file is provided in Appendix A and is also archived with the model code available for download at the Exponent CALPUFF website (www.src.com). Appendix B contains information on re-compiling the model FORTRAN code on both Windows and LINUX platforms.

1 Processing Options

CALNO2 is built to perform the calculations necessary for the ARM and OLM methods. The first section of the code requires the user to select the processing mode (MODE=1 for ARM and MODE=2 for OLM). This section of the input control file is presented in Table 1-1.

Depending on the option selected, additional parameters will need to be specified in Section 2 and Section 3 of the input control file.

Table 1-1 CALNO2 Input File – Section 1. Processing Options

```
Section 1.  Processing Options
-------------------

   Select NOx to NO2 processing option.  Ambient Ratio Method (ARM) will convert
   NOx based on a pre-defined concentration-based polynomial. Ozone Limiting Method
   (OLM) will convert based on stack specific NO2/NOx ratios and hourly ambient
   ozone concentrations contained in either an external ozone.dat file or monthly
   ozone concentrations defined below.

   NOx to NO2 conversion methodology                 No Default  ! MODE =  1  !
       1 = Ambient Ratio Method (ARM)
       2 = Ozone Limiting Method (OLM)
```

2 ARM Options

Table 2.1 contains the input file variables for Section 2 – ARM Options. The Ambient Ratio Method calculates NO_x concentration using specific NO_2 to NO_x conversion ratios. In CALNO2 these conversion ratios can be applied based on 6 different internally defined 6th order polynomials of the form:

$$NO_2/NO_x = C_0 + C_1 \cdot NO_x + C_2.NO_x^2 + C_3 \cdot NO_x^3 + C_4 \cdot NO_x^4 + C_5 \cdot NO_x^5 + C_6 \cdot NO_x^6$$

or based on a user defined exponential function of the form:

$$NO_2/NO_x = A \cdot NO_x^b$$

The 6 internally defined 6th order polynomials use constants defined by BCENV for 5 different categories of landuse (all, urban, rural, industrial, and coastal) plus the values for the USEPA's ARM2 equation as defined in the AERMOD model. The constants used for each equation are listed in Table 2-2 and are based on values contained in the British Columbia NO_2 Guidance Document. In Input Section 2 of the CALNO2 control file, the user must select a value defining the profile selected. Values of APROF = 1 through 6 represent the 6 internally defined polynomial equations. Selecting APROF = 7 allows the user to define an exponential equation with subsequent variables defining the prefactor (AFACT) and exponential (BFACT) to be used based on the equation listed above.

Because ARM is not dependent on the source contribution of each stack, there is no requirement for the CALPUFF to be run with individual stacks modeled separately or to use the MSOURCE=1 option in CALPUFF. While separate runs and source contributions are acceptable, they are not necessary and CALNO2 will process a single run that contains only the total contribution of all sources.

Table 2-1 CALNO2 Input File – Section 2. ARM Options

```
Section 2.  ARM Options:
------------

    Specify the NO2/NOx conversion profile to be used
    [Required if ARM Method is selected MODE = 1]

      1 = BC Profile for All Regions                No Default  ! APROF =  1  !
      2 = BC Profile for Urban Regions
      3 = BC Profile for Rural Regions
      4 = BC Profile for Industrial Regions
      5 = BC Profile for Coastal Regions
      6 = USEPA Profile
      7 = User Defined Exponential profile (Ax^b)

    User Defined Exponential Profile
    Define constants for an exponential profile of the form:
      (A * NOx^b)
    Required if ARM Method MODE = 1 selected with User Defined Profile APROF = 7
       No Default

          ! AFACT = 10.0 !
          ! BFACT = -0.6 !
```

Table 2-2 ARM Curve 6th Order Polynomial Equation Coefficients (µg/m^3)

Polynomial	BC-Specific ARM2 Curves					U.S EPA
Order	All	Urban	Rural	Industrial	Coastal	Default
0	1.4217E+00	1.4081E+00	7.0908E-01	9.7054E-01	1.4097E+00	1.2441E+00
1	-9.0043E-03	-8.4309E-03	1.8014E-02	2.7563E-03	-8.6617E-03	-2.7383E-03
2	2.8689E-05	2.2008E-05	-4.0219E-04	-8.0316E-05	2.6443E-05	-5.6062E-06
3	-5.1310E-08	-1.8692E-08	3.1248E-06	4.4204E-07	-5.9049E-08	3.4555E-08
4	6.2556E-11	-1.4082E-11	-1.1639E-08	-1.0885E-09	1.3159E-10	-5.8345E-11
5	-5.5299E-14	2.9761E-14	2.0910E-11	1.2663E-12	-2.0684E-13	4.2795E-14
6	2.4169E-17	-1.1526E-17	-1.4534E-14	-5.6578E-16	1.3132E-16	-1.1723E-17

3 OLM Options

The Ozone Limiting Method will perform conversion from NO_x to NO_2 based on the amount of available ozone. If OLM (MODE=2) is selected, the method requires the user to define stack specific in-stack ratios (NO_2/NO_x), the atmospheric NO_2/NO_x equilibrium ratio, and the source of ozone data to be used in the ozone limiting calculations.

Table 3-1 contains the input variables for Section 3 – OLM Options. The user must define the total number of sources included in the CALPUFF concentration files (NSOURCE). These sources may be spread across multiple concentration files, but if more than one source is included in a single CALPUFF concentration file, then the CALPUFF run must have been performed to save source contributions (MSOURCE=1). This provides a list of source names (SRCNAME) and associated NO_2/NO_x in-stack ratios ($NO2NO_x$) for each modeled source. There must be one value for each modeled source and all source names must match exactly with the source names listed in the associated CALPUFF runs. A fatal error will be produced by the CALNO2 code if there is any mismatch between source names or the number of sources. An equilibrium ratio is defined (EQUIL) which represents the maximum equilibrium $NO2/NO_x$ ratio in the atmosphere.

CALNO2 will calculate the amount of NO_2 emitted on a stack-by-stack basis based on the provided in-stack ratio (NO_2/NO_x) values. The balance of the emitted NO_x (treated as NO) will be converted to NO_2 at each receptor based on the ratio of moles of ozone to moles of NO. The CALNO2 input file allows the user to define whether the conversion limit is calculated based on the summed concentration over all stacks such that the stacks are competing for available ozone (OCOMP=1) or if each stack individually sees the full available ozone and separate stacks do not compete (OCOMP=2). An individual run of CALNO2 must have all stacks either competing or not competing. If the user desire is to have separate groups where stacks only compete among the group, this can be accomplished by running CALNO2 separately for each group of stacks and then combining the results using CALSUM or POSTUTIL. The use of separate CALNO2 runs would also allow for the specification of different background ozone values for each group.

Background ozone values are required to calculate the amount of NO converted to NO_2. These values can be specified in one of two methods. An hourly ozone file can be used to specify ozone concentrations during each hour (OZSRC=1). If selected, the name of the ozone file will be specified using the variable OZFILE and the file format is the same as specified for use in Version 7 of the CALPUFF model. Table 3-2 includes a sample of this OZONE.DAT format and the file variables are defined in Table 3-3 through Table 3-5. For use with CALNO2, the OZONE.DAT file must include individual records for each 1-hour time period. If missing hourly records occur in the data file, they must be filled by the user prior to running CALNO2. Additionally, even though the OZONE.DAT format will allow specification of data for more than one ozone station, only the first station will be used by CALNO2 when calculating NO_x to NO_2 conversion.

Table 3-1 CALNO2 Input File – Section 3. OLM Options

```
Section 3.  OLM Options:
------------

   Number of CALPUFF concentration files.       No Default  ! NSOURCE = 3 !
   Note: all files processed must contain
   the same time period and receptors. If
   selecting OLM (MODE=2) each CALPUFF run that contains
   multiple sources must have been run with MSOURCE=1
   in order to save source contributions.

   For each source contained in the CALPUFF files, specify the
   source name from the CALPUFF run and the in-stack NO2/NOx ratio
   for the stack (value between 0.0 and 1.0)
   [Must include NSOURCE uniquely named entries]
   [Only used if OLM is selected MODE = 2]

               SRCNAME, NO2/NOx
       -------    --------------
      ! NO2NOX  = SRC1, 0.10 !
      ! NO2NOX  = SRC2, 0.20 !
      ! NO2NOX  = SRC3, 0.30 !

   NO2/NOx ambient equilibrium ratio            Default: 0.9     ! EQUIL = 0.9 !

   Do all sources compete for ambient ozone     Default = 1      ! OCOMP = 1 !
      1 = All sources compete for ambient ozone
      2 = Each source sees full ambient ozone

   Specify the method for providing background ozone concentrations

      1 = hourly ozone.dat file                   No Default  ! OZSRC =  1  !
      2 = monthly ozone values (defined below)

   Ozone file containing hourly ozone concentrations
   only the first ozone station included in the file will be used
   to convert NOx to NO2.
   Required if OLM Method is selected MODE = 2 with hourly ozone inputs OZSRC = 1

          ! OZFILE = ozone.dat  !

   Monthly ozone concentrations (micrograms/m3)
   Required if OLM Method is selected MODE = 2 with monthly ozone inputs OZSRC = 2

          ! OZJAN = 80.0 !
          ! OZFEB = 80.0 !
          ! OZMAR = 80.0 !
          ! OZAPR = 80.0 !
          ! OZMAY = 80.0 !
          ! OZJUN = 80.0 !
          ! OZJUL = 80.0 !
          ! OZAUG = 80.0 !
          ! OZSEP = 80.0 !
          ! OZOCT = 80.0 !
          ! OZNOV = 80.0 !
          ! OZDEC = 80.0 !
```

Table 3-2 Example Hourly Ozone File (OZONE.DAT)

```
OZONE.DAT 2.1 Comments, times with seconds, time zone, coord info
1
Prepared by user
UTM
11N
NWS-84 02-21-2003
KM
UTC-0800
2016 365 23 0000 2017 001 17 3600
1
'STATION 1' 168.000 3840.000
2016 365 23 0000 2016 365 23 3600 66.
2017 001 00 0000 2017 001 00 3600 65.
2017 001 01 0000 2017 001 01 3600 68.
2017 001 02 0000 2017 001 02 3600 66.
2017 001 03 0000 2017 001 03 3600 65.
2017 001 04 0000 2017 001 04 3600 67.
2017 001 05 0000 2017 001 05 3600 72.
2017 001 06 0000 2017 001 06 3600 70.
2017 001 07 0000 2017 001 07 3600 69.
2017 001 08 0000 2017 001 08 3600 72.
2017 001 09 0000 2017 001 09 3600 74.
2017 001 10 0000 2017 001 10 3600 87.
2017 001 11 0000 2017 001 11 3600 102.
2017 001 12 0000 2017 001 12 3600 109.
2017 001 13 0000 2017 001 13 3600 120.
2017 001 14 0000 2017 001 14 3600 116.
2017 001 15 0000 2017 001 15 3600 103.
2017 001 16 0000 2017 001 16 3600 98.
2017 001 17 0000 2017 001 17 3600 89.
```

Table 3-3 OZONE.DAT Header Record Variables

OZONE.DAT 2.1 Comments	Dataset Name, Dataset Version, Dataset Message (char*16, char*16, char*64) **Format: (2a16, a64)**
1	Number of comment lines to follow (integer) **Free-Format**
Comment Line 1	Comment lines (80 characters per record are read)
UTM **11N**	Map Projection Type (char*8) **Format: (a8)** UTM Zone, Hemisphere (integer, char*1) **Format: (i4, a4)** *[See Table 3-5 for alternate map projection records]*
NAS-C 02-21-2003	DATUM code and date (char*8, char*12) **Format: (a8, a12)**
KM	Map units are kilometers (char*4) **Format: (a4)**
UTC-0800	Time Zone as (UTC+hhmm) (char*8) **Format: (a4)**
2016 365 23 0000 2017 001 17 3600	Start time and end time of data in file as Year, Julian Day, Hour, Second (0-3599) (integer) **Free-Format**
1	Number of ozone station (only one will be read) **Free-Format**
'STATION 1' 168.000 3840.000	Station name (char*16), East Coord, North Coord **Free-Format (single quotes required for station name)**

Table 3-4 OZONE.DAT Map Projection Records

UTM **19N**	**Universal Transverse Mercator** Map Projection Type (char*8) **Format: (a8)** UTM Zone, Hemisphere (integer, char*1) **Format: (i4, a4)**
LCC **40.5N 90.0W 30.0N 60.0N** **0.00000000E+00 0.00000000E+00**	**Lambert Conformal Conic** Map Projection Type (char*8) **Format: (a8)** Origin Latitude, Origin Longitude, and two matching parallels (char*16) **Format: (4a16)** False Easting and Northing km (real) **Free-Format**
TTM **40.5N 90.0W** **0.00000000E+00 0.00000000E+00**	**Tangential Transverse Mercator** Map Projection Type (char*8) **Format: (a8)** Origin Latitude, Origin Longitude (char*16) **Format: (2a16)** False Easting and Northing km (real) **Free-Format**
PS **40.5N 90.0W 30.0N**	**Polar Stereographic** Map Projection Type (char*8) **Format: (a8)** Origin Latitude, Origin Longitude, and 1 matching parallel (char*16) **Format: (3a16)**
EM **0.0N 90.0W**	**Equatorial Mercator** Map Projection Type (char*8) **Format: (a8)** Origin Latitude, Origin Longitude (char*16) **Format: (2a16)**
LAZA **40.5N 90.0W** **0.00000000E+00 0.00000000E+00**	**Lambert Azimuthal Equal Area** Map Projection Type (char*8) **Format: (a8)** Origin Latitude, Origin Longitude (char*16) **Format: (2a16)** False Easting and Northing km (real) **Free-Format**

Table 3-5 OZONE.DAT Time-Varying Data Records

2002 009 00 0000 2002 009 05 0000 80 **2002 009 05 0000 2002 009 06 0000 81** **2002 009 06 0000 2002 009 20 0000 82**	Time Period 1 to N (spanning start to end time in file): Period start and end times (integers) Start Year, Julian Day, Hour, Second(0-3599), End Year, Julian Day, Hour, Second(0-3599) Ozone Concentration (ppb) **Free-Format**
• While more than one Ozone station can be included in the file format, only the first will be used for CALNO2 processing. • Missing Ozone values should be filled by the user prior to processing with CALNO2	

4 Input Files

Section 4 of the CALNO2 input file includes a list of CALPUFF concentration files which will be processed. These concentration files do not need to be in a specific order, but if OLM has been selected, Section 3 of the input control file must provide in-stack ratio values for each stack and the concentration files need to include source contributions from each stack. This can be accomplished either by running individual stacks in separate runs, or by using the MSOURCE=1 option in CALPUFF which will save individual stack source contributions. CALNO2 will accept any combination of single source runs with MSOURCE=0 and single or multiple source runs with MSOURCE=1. NO_x concentrations in the specified files will be processed to calculate NO_2. All other species will be summed.

The input CALPUFF concentration files listed must exactly match the following run parameters. Any mismatches will result in an error when running CALNO2.

- The number of gridded, discrete and complex terrain receptors
- The grid datum and projection
- The beginning and ending time of the runs
- The run time zone
- The species modeled

Table 4-1 CALNO2 Input File – Section 4. Input Files

```
Section 4.  Input Files
-----------

   Provide one or more filenames for CALPUFF concentration files to process
   (place assignments between delimiters):

      ! INPFILE = source1.con !
      ! INPFILE = source2.con !
      ! INPFILE = source3.con !
```

5 Output Files

CALNO2 will produce two output files, 1.) a new CALPUFF format binary concentration file (BINFILE) and 2.) a list file (LSTFILE) which documents model options selected and any errors or warnings produced by the CALNO2 code. The new CALPUFF binary concentration will contain the total NO_2 concentration at each receptor (both gridded and discrete) as calculated using ARM or OLM. For any species other than NO_x that are contained in the input concentration files, the output file will contain the sum of all stacks at each modeled receptor.

Table 5-1 CALNO2 Input File – Section 5. Output Files

```
Section 5.  Output Files
------------

   Binary CALPUFF-format file containing NO2 concentrations:
     File name                 No Default             ! BINFILE = calno2.con !

   Name of output list file for run:
     List-file name            Default: CALNO2.LST    ! LSTFILE = calno2-test.lst !

   All file names will be converted to either lower or upper case
         T = lower case       (LCFILES)    Default: F     ! LCFILES = F !
         F = UPPER CASE
```

Appendix A

Sample CALNO2.INP

CALNO2.INP

```
CALNO2.INP      7.0            DEMO Configuration
--------------------------------------------------------------------------------

                    CALNO2 Processor CONTROL FILE
                    -----------------------------
PURPOSE
-------

This utility reads a set of CALPUFF-format output files (CONC)
and convert modeled NOx to NO2 based on one of two methods: Ambient Ratio Method
or Ozone Limiting Method.  The resultant concentration file will replace
modeled NOx concentrations with converted NO2 concentrations.

--------------------------------------------------------------------------------

  Section 1.  Processing Options
  ------------------

     Select NOx to NO2 processing option.  Ambient Ratio Method (ARM) will convert
     NOx based on a pre-defined concentration based polynomial. Ozone Limiting Method
     (OLM) will convert based on stack specific NO2/NOx ratios and hourly ambient
     ozone concentrations contained in either an external ozone.dat file or monthly
     ozone concentrations defined below.

     NOx to NO2 conversion methodology                 No Default  ! MODE =  1  !
         1 = Ambient Ratio Method (ARM)
         2 = Ozone Limiting Method (OLM)

  Section 2.  ARM Options:
  ------------

      Specify the NO2/NOx conversion profile to be used
      [Required is ARM Method is selected MODE = 1]

        1 = BC Profile for All Regions                          No Default  ! APROF =  1  !
        2 = BC Profile for Urban Regions
        3 = BC Profile for Rural Regions
        4 = BC Profile for Industrial Regions
        5 = BC Profile for Coastal Regions
        6 = USEPA Profile
        7 = User Defined Exponential profile (Ax^b)

      User Defined Exponential Profile
      Define constants for an exponential profile of the form:
        (A * NOx^b)
      Required if ARM Method is selected MODE = 1 with User Defined Profile APROF = 7]
         No Default

            ! AFACT = 10.0 !
            ! BFACT = -0.6 !

  Section 3.  OLM Options:
  ------------

     Number of CALPUFF concentration files.       No Default  ! NSOURCE = 3 !
     Note: all files processed must contain
     the same sources and receptors. If
     selecting OLM (MODE=2) each CALPUFF run that contains
     multiple sources must have been run with MSOURCE=1
     in order to save source contributions.

     For each source contained in the CALPUFF files, specify the
     Source name from the CALPUFF run and thein-stack NO2/NOx ratio
     For the stack (value between 0.0 and 1.0)
     [Must include NSOURCE uniquely named entries]
     [Only used if OLM is selected MODE = 2]

                    SRCNAME, NO2/NOx
         -------    --------------
        ! NO2NOX  = SRC1, 0.1 !
        ! NO2NOX  = SRC2, 0.2 !
```

```
      ! NO2NOX  = SRC3, 0.3 !

    NO2/NOx ambient equilibrium ratio            Default: 0.9     ! EQUIL = 0.9 !

    Do all sources compete for ambient ozone     Default = 1      ! OCOMP = 1 !
       1 = All sources compete for ambient ozone
       2 = Each source sees full ambient ozone

    Specify the method for providing background ozone concentrations

       1 = hourly ozone.dat file                   No Default  ! OZSRC =  1  !
       2 = monthly ozone values (defined below)

    Ozone file containing hourly ozone concentrations
    only the first ozone station included in the file will be used
    to convert NOx to NO2.
    Required if OLM Method is selected MODE = 2 with hourly ozone inputs OZSRC = 1

           ! OZFILE = ozone.dat  !

    Monthly ozone concentrations (micrograms/m3)
    Required if OLM Method is selected MODE = 2 with monthly ozone inputs OZSRC = 2

           ! OZJAN = 80.0 !
           ! OZFEB = 80.0 !
           ! OZMAR = 80.0 !
           ! OZAPR = 80.0 !
           ! OZMAY = 80.0 !
           ! OZJUN = 80.0 !
           ! OZJUL = 80.0 !
           ! OZAUG = 80.0 !
           ! OZSEP = 80.0 !
           ! OZOCT = 80.0 !
           ! OZNOV = 80.0 !
           ! OZDEC = 80.0 !

Section 4.  Input Files
-----------

   Provide one or more filenames for CALPUFF files to process
   (place assignments between delimiters):

      ! INPFILE = source1.con !
      ! INPFILE = source2.con !
      ! INPFILE = source3.con !

Section 5.  Output Files
------------

   Binary CALPUFF-format file containing NO2 concentrations:
     File name                   No Default              ! BINFILE = calno2.con !

   Name of output list file for run:
     List-file name              Default: CALAVE.LST     ! LSTFILE = calno2-test.lst !

All file names will be converted to either lower or upper case
         T = lower case       (LCFILES)    Default: F     ! LCFILES = F !
         F = UPPER CASE
```

Appendix B

Example Compilation Statements

```
Compiling and linking with CALNO2 using Lahey LF95 for Windows

lf95 modules.for calno2.for -o0 -sav -co  -trap doi -out calno2.exe >cpl.txt

del *.obj
del *.map
del *.mod

Switch settings ------------------------------
-o0          No optimization
-co          Display the compiler options that are used
-sav         Save local variables
-trap doi    Trap NDP divide-by-zero (d), overflow (o), and invalid operation (i)
-out         Name the compiled executable to "calmax.exe"
>cpl.txt     Send compiler screen output to file "cpl.txt"
```