BolChem 0.9

A 3D Prediction Model of the Meteorology and the Chemical Composition of the Atmosphere

project documentation

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Abstract

With this project a model to predict the meteorology and the chemical composition of the atmosphere is provided. Two existing codes, `Bolam` [4] for the meteorology and `UAM-IV` [1] extended by the SAPRC mechanism [3] for the chemical part, were adapted and an interface was constructed on the base of the *FCM* interface [5].

Contents

Chapter 1

Chemistry

To insert the chemical processor into the meteorological solver `Bolam` the *FCM* interface (Flexible Chemical Mechanism)[5] was used, while the chemical processor itself is based on the integration scheme of `UAM-IV` [1].
Roughly the procedure can be described as follows:

- All input files, initialisation and boundary fields are read in by `Bolam`, also the chemistry files.
- All necessary fields are initialised.
- The meteorological processor is called, performing advection, diffusion and time integration of the meteorological variables, as in the standard version of `Bolam` [4].
- the chemical processor is called. It performs:
  - the horizontal diffusion scheme and the advection scheme of `Bolam` adapted for the concentrations of the involved species.
  - the vertical diffusion, as in `UAM-IV`[1].
  - the computation of the surface fluxes of the chemical species, as in `UAM-IV`.
  - the time integration of slow and fast chemical reactions as in `UAM-IV`.

For the moment the whole interface works in one direction only, in the sense that the meteorological solver passes the updated variables to the chemical processor, which, on the base of these, defines the actual ambient for the chemical reactions and updates the concentration field, while the meteorological variables remain untouched of the chemical reactions, such that the effect of the atmospheric dynamics on the chemistry is accounted for, while the effect of the chemical reactions on the meteorological state of the atmosphere is ignored.
Figure 1.1 gives a flux diagram of the chemical processor.

1.1 Time Integration

The time integration scheme of the chemical part allows as input an arbitrary time step, which is then subdivided automatically by the numerical routines

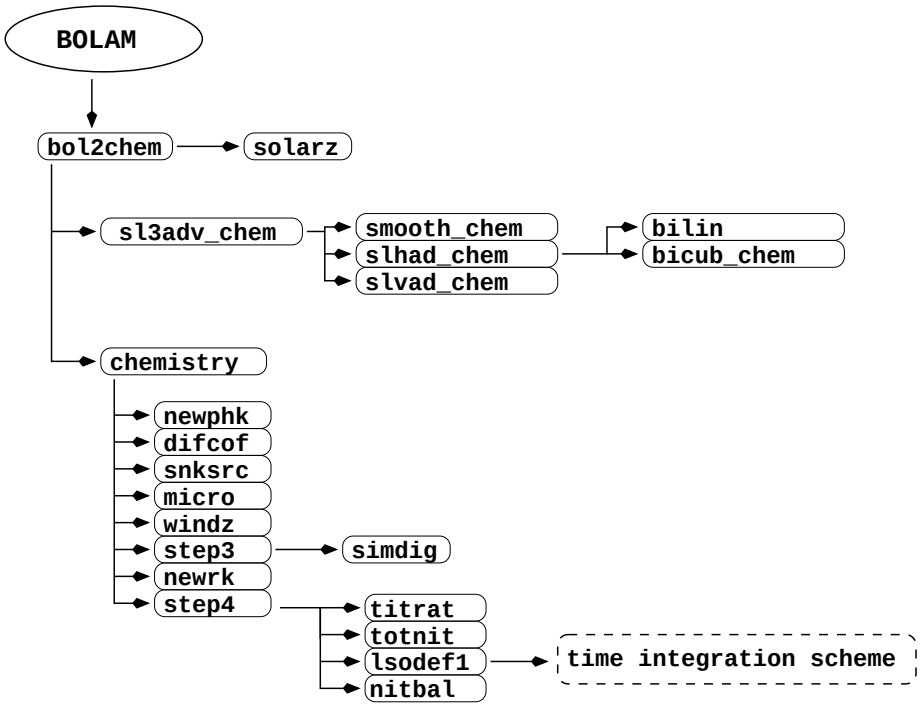

Figure 1.1: The Program Flux of the Chemical Processor

of the chemical part itself in relation to the chosen mechanism (as described in [5]). The time step of `Bolam` could therefore be passed to the chemistry without worrying about its adaptation to the reaction rates. (For the treatment of the time integration in `Bolam` see [4].) A jumper `NTGL` was inserted into `bolchem.inp` to call the chemistry processor only every `NTGL` time steps.
It could be useful for the future to insert a re-adaption of `NTGL` in relation to the time-steps performed by the chemical solver.

1.2 Peculiarities of the Interface

- The z(σ)-direction in `Bolam` is opposite to the z-direction in the chemical solver.
- The Advection in the chemical solver is calculated in σ (`slvad.f`), diffusion in z (`difcof.f`, `step3.f`).
- The velocities passed from `Bolam` are given in $\frac{m}{s}$, while the chemical solver uses $\frac{m}{h}$.
- The time step passed from `Bolam` is given in s, while the chemical solver uses h or min.
- To ensure the conservation of mass in the chemical solver a tracer gas (calibration gas) is used as an additional species.
- Two variables are used in the code to indicate the no. of chemical species:

  - `NOSPEC`: Actual number of species for used mechanism, read from mechanism file `chemparm` (tracer gas excluded).
  - `NSMAX`: Maximum no. of species for dimensions of several `ARRAYS` of the chemical solver, defined in `chparm.cmd` (tracer gas included).

  They should contain corresponding values, which is assured by the chemical preprocessor.

- `kbeg` is set to 1.→ The surface layer is not separated from vertical column.
- Through the entire program including *I/O*-procedures `BolChem` works with concentrations in *ppm*, except for the tracer gas in the internal of the program which is given in unit 1.

1.3 Unsupported Features

- The input for the stability model of the chemical processor used in `difcof.f` has to be provided (i.e. level of the diffusion break, exposure class), or preferably a more recent model should be inserted. (For more details on the implemented model, see [1, 2])
- The I/O-Routines for Emissions (`qt`) are not prepared yet, emissions are set to 0.
- The concentrations on top of the region are for the moment considered to be constant in time.
- Point Sources are for the moment not supported, though their use is partially prepared (see `step3.f`). To include them, pass the point source emissions and a switcher to `step3.f`, uncomment the necessary lines (using a switcher, only `qpts` is needed of the old stuff!) and prepare I/O of point source emissions.

1.4 Variables Passed from `Bolam` to the Chemical Processor

- `conc:common.chem - NLON, NLAT, NLEV, NSMAX` field of the concentrations of each species

  `bol2chem.f`

  `chemical.f:conc(nx,ny,nz,nspec)`

  `sl3dadv.f:conc(NLON,NLAT,NLEV)`

- `NLON:dimensioni_bolchem` dimension in longitudinal direction

  `bol2chem.f`

  `chemical.f:nx`

  `sl3dadv.f`

  `windz.f:nx`

- NLAT:dimensioni_bolchem dimension in latitudinal direction
  - bol2chem.f
  - chemical.f:ny
  - sl3dadv.f
  - windz.f:ny
- NLEV:dimensioni_bolchem dimension in vertical direction
  - bol2chem.f
  - chemical.f:nz
  - sl3dadv.f
  - difcof.f:nz
  - windz.f:nz
  - step3.f:nz
- NOSPEC:chparm.cmd actual no. of species from chemparm
  - chemical.f:nspec
  - micro.f:nspec
  - step3.f:nspec
- DTSTEP:common.all time step in seconds
  - bol2chem.f:dtmeteo
  - chemical.f:dtmeteo
  - micro.f:dt
  - step3.f:dt
  - step4.f:dt
  - windz.f:dt
- U:common.all - NLON, NLAT, NLEV longitudinal velocity
  - bol2chem.f
  - chemical.f:U(nx,ny,nz)
- V:common.all - NLON, NLAT, NLEV latitudinal velocity
  - bol2chem.f
  - chemical.f:V(nx,ny,nz)
- PS:common.all - 1:NLONP1, 0:NLAT $\rightarrow$ pressure field: $P = P_s * \sigma$
  - bol2chem.f:P(NLON,NLAT,NLEV)
  - chemical.f:P(nx,ny,nz)
- T:common.all - NLON, NLAT, NLEV
  - bol2chem.f
  - chemical.f:T(nx,ny,nz)
  - step3.f:T(nz)
  - newrk.f:tempr
  - step4.f:tcll

- `bustar:bolcp.cmd - NLON,NLAT` friction velocity

  `bol2chem.f`

  `chemical.f:ustar:cntrol.cmd`

  `difcof.f:ustar:cntrol.cmd`

  `micro.f:ustar:cntrol.cmd`

- `BRGM:bolcp.cmd - NLON, NLAT` roughness for momentum diffusion

  `bol2chem.f:rough(nx,ny)`

  `chemical.f:rough(nx,ny)`

  `difcof.f:rough`

- `frvis:common.all - NLON,NLAT` visible radiation

  `bol2chem.f`

  `chemical.f:frd(nx,ny`

- `PHIH(NLON,NLAT,NLEV)` geopotential → thickness of vertical cells

  `bol2chem`

  `chemical.f:th(nz)`

  `difcof.f:th(nz)`

  `windz.f:th(nz)`

  `step3.f:th(nz)`

- `VEGETA(NLON,NLAT)` vegetation factor

  `bol2chem.f:vegeta`

  `chemical.f:veg(nx,ny)`

  `snksrc.f:veg`

1.5 The Chemical Preprocessor

The program was established on the SAPRC mechanism [3] and includes already all the files necessary for this mechanism. Nevertheless, it is possible to change this mechanism; in this case the chemical preprocessor has to be rerun. Its usage is well explained in [5].
Small changes were applied to the source-files of the preprocessor, basically to change the usual `FORTAN` include-statement into the c-preprocessor statement.
On runtime the species record of the chemical input file `chemparm` is checked back with the species record defined by the preprocessor, editing of this record in `chemparm` only will lead to errors and the program exits!
The preprocessor files are designed to be compiled using *absoft*'s `f77` Compiler and its libraries (while `BolChem` is designed for the GNU-`g77` Compiler).

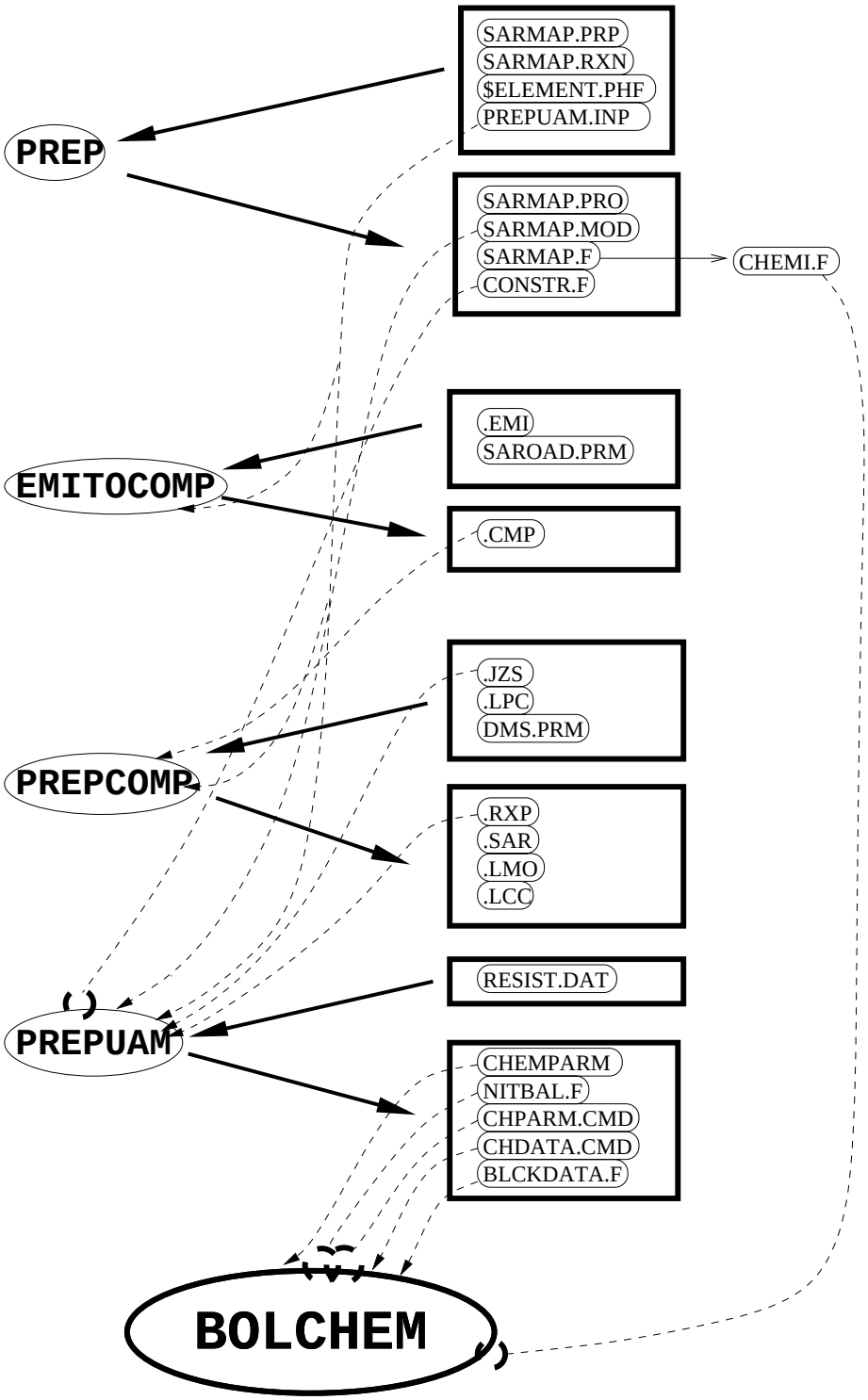

Figure 1.2: The Chemical Preprocessor

Chapter 2

Comments on Bolam and its modifications

In the realization of the interface between the meteorological and the chemical part of BolChem the following modifications were applied to the original code of Bolam:

- A new COMMON block bolcp.cmd was included containing the ARRAY bustar to pass the friction velocity u_* from SUBROUTINE VDIFF to the chemical processor.
- The unit indicators for the chemical I/O-files were added to the NAMELIST MODEL and common.all , see *chapter 3*.
- The variable frdark, giving the lower radiation limit for photolytic reactions, was added to the NAMELIST MODEL and common.all.
- The relative and absolute error tolerances for the chemical solver were added to the NAMELIST MODEL and common.all.
- A jumper to call the chemical solver every NTGL steps of Bolam's timestep was added to the NAMELIST MODEL and common.all.
- The OPEN-option POSITION='APPEND' was removed and replaced by manual forwarding for compatibility with standard FORTRAN.
- The calls of chemical i/o-routines were added. For that purpose also the routine wrhist.f was supplemented and moved to an external file.

For a correct implementation of the radiation SUBROUTINE radial.f, the variables of type REAL in this routine have to be compiled in double precision! (Realized by using the f2c-compiler, see D.4.)

Chapter 3

The I/O mechanism

The I/O structure of `Bolam` (in detail described in [4]) was supplemented to include reading and writing of the concentration field, as well as of the data of the involved chemical mechanism and interface parameters. In detail the following modifications were applied:

- A file format *CHF* was created to initialise the concentrations, set the boundary values and write the history file, corresponding to the *MHF* format of `Bolam` (see [4], chapter B.3). The routines are called corresponding to the *MHF*-calls. The associated unit indicators are:
  - `NUNICC`: no. of chemical ic-file, corr. to NUNIC, defined in `bolchem.inp`, by default set to 31.
  - `NUNBCC`: no. of chemical bc-file, corr. to NUNBC, defined in `bolchem.inp`, by default set to 31.
  - `IUNBCC`: no. of successive chemical bc-file, corr. to IUNBC, for now not supported!
  - `NUNHC`: no. of chemical history file, corr. to NUNHI, defined in `bolchem.inp`, by default set to 30.

  By default the first boundary file and the initialisation file are one, either for the meteorological variables, either for the concentrations of the species.
- `UAM-IV`'s `chread.f` routine was included with the unit indicators:
  - `NCINP` for `chemparm`, by default set to 29.
  - `NCTRC` for `simcontrol`, by default set to 28.
- The modified `WRHIST` definition was moved to an own file `wrhist.f`
- The `Bolam` formats *rf* and *mpg* are not supported.
- For the moment no time dependent chemical boundary values.
- Some parameters were added to the `NAMELIST MODEL` and to the input file `bolchem.inp` (see appendix C.2)

- All the unit indicators concerning concentration fields and chemical parameters.
- The limiter `FRDARK` for photolytic reactions.
- Absolute and relative error tolerances for the chemical solver.
- A jumper for the call of the chemical solver.

Chapter 4

User's Guide

4.1 The Geometry

`BolChem` 's geometry is defined in the file `dimensioni_bolchem` and in the *FDR* and *PDR* records of `Bolam`'s *MHF* files. They contain the longitudinal, latitudinal and vertical dimensions, first longitude and latitude and their increments as well as the sigma levels. Take care that the dimensions of the *FDR* record are the same as in `dimensioni_bolchem` and remember that the σ-index starts at the top of the domain and increases downward! (For more details, see [4].)

4.2 Preprocessing before Compilation

The geometrical dimension and the chemical mechanism of the model have to be defined before compilation, as a consequence any changes to those objects claim recompilation!
The geometrical dimension is defined in a file called `dimensioni_bolchem`, see appendix C.1. It is edited to the preferred dimension and has to be placed in the main source directory `/bolchem/src/`.
The chemical mechanism is defined by the chemical preprocessor, described in chapter 1.5 and [5]. It provides the source files `nitbal.f`, `blckdata.f` and `chemi.f` and the `include` files `chparm.cmd` and `chdata.cmd`. These files have to be copied into the chemical source directory`/bolchem/src/chemistry/` before compiling.
In addition the input file `chemparm` is created. It is needed to run `BolChem` after compilation.
The standard mechanism is the SAPRC mechanism [3]. The present files represent this mechanism and no further chemical mechanism preprocessing is needed, if SAPRC shall be used!
The files defining the chemical mechanism shouldn't be edited manually, but generated with the mentioned preprocessor!

4.3 Compilation

The source files are organised in three directories, which are:

- `/bolchem/src/`: containing `Bolam`'s source files.
- `/bolchem/src/radiation/`: containing `Bolam`'s radiation routine.
- `/bolchem/src/chemistry/`: containing the source files of the interface and the chemical processor.

Each directory has its `Makefile` (given in appendix D), involved by the main `Makefile` in `/bolchem/src/`, so to compile the whole program just call the main `Makefile` in `/bolchem/src/`. `make install` will copy the executable into `/bolchem/` and link it to the local `/bin/`-directory.

4.4 Preprocessing after Compilation

The executable of `BolChem` needs the following input fields to run:

- `chemparm`: contains the input parameters for the chemical mechanism.
- `fort.41`, ...(default name): contains descriptor records and meteorology initialisation and successive boundary conditions.
- `fort.31` (default name): contains descriptor records, the initialisation and boundary conditions of the concentration fields.
- `bolchem.inp`: contains control parameters of the simulation.

`chemparm` is generated automatically by the chemical preprocessor as described above.
The meteorological boundary and initialisation files can be generated with the standard-`Bolam` preprocessor. Take care that the dimensions applied correspond to the ones in your `dimnesioni_bolchem`!
The concentration initialisation has to be done in the newly defined *CHF* format. To create this format you can use the routine `wcinit.f` given in appendix E. The descriptor records of the chemistry initialisation file is a dummy and is not read in by `BolChem` . It was included to make possible a more direct usage of a solution file `bolchem.chf` as initialisation.
The `bolchem.inp` file is edited manually. An example file is given in appendix C.2, which also contains an explanation of all its parameters. For more details see [4].

4.5 Running `BolChem`

All files of the preprocessing after compilation have to be copied into the directory from where `BolChem` is executed. If the executable is not included in the default `PATH` also it also has to be copied here. Then the program can be run by simply calling the executable.

Appendix A

List of Files

A.1 Source Files

A.1.1 `Bolam`

- `bolam.f` - main program and several subroutines
- `convec.f` - computes deep convection, called subroutines included
- `radial.f` - radiation subroutine
- `wrhist.f` - routine managing output calls

A.1.2 Chemical Processor

- `bicub.f` - bilinear interpolation
- `bilin.f` - bicubic interpolation
- `blckdata.f` - data block with chemical species
- `bol2chem.f` - routine dealing the interface of `Bolam` and the chemical processor, called by `Bolam`
- `chemi.f` - computes rates for the preprocessed mechanism
- `chemical.f` - chemical frame (subroutine `CHEMISTRY`
- `chread.f` - chemical input routine
- `difcof.f` - computes momentum diffusion coefficients for vertical column
- `io_chf.f` - i/o routines of chemical data
- `lsfun.f` - numerical routines
- `lsodef1.f` - *DGL*-solver
- `micro.f` - flux of species from the surface
- `newphk.f` - photolysis rates
- `newrk.f` - calculates rates temperature dependent rate constants

- `nitbal.f` - nitrogen balance
- `simdig.f` - solver for tridiagonal systems
- `sl3dadv.f` - advection frame
- `slhad.f` - horizontal advection
- `slvad.f` - vertical advection
- `smooth.f` - horizontal diffusion
- `snksrc.f` - deposition velocity and sources
- `steady.f` - steady state values of NO, NO_2, O_3
- `step3.f` - spatial integration in z direction
- `step4.f` - chemical core with time integration
- `stodef1.f` - numerical routine
- `titrat.f` - steady-state concentration of NO, NO_2, NO_3 and O_3 at night by mathematical titration
- `windz.f` - vertical winds

A.2 Files Included before Compilation

A.2.1 `Bolam` and `bol2chem.f`

- `common.all` - `Bolam`'s `COMMON` block
- `dimensioni_bolchem` - geometrical dimensions
- `bolcp.cmd` - `COMMON` block with friction velocity u_*
- `common.chem` - `COMMON` block with concentration field

A.2.2 Chemical Processor

- `balanc.cmd` - `COMMON` block for mass fluxes across boundaries
- `calib.cmd` - `COMMON` block with name of calibration gas and subscript
- `chdata.cmd` - `COMMON` block with species data for preprocessed mechanism
- `chparm.cmd` - `COMMON` block with chemistry parameters and parameter field declarations
- `cntrol.cmd` - `COMMON` block with dimension and region descriptors
- `common.chem` - `COMMON` block with concentration field
- `filcon.cmd` - `COMMON` block with file control variables
- `locptr.cmd` - `COMMON` block with pointers to local variables of the integration scheme

- `mscal.cmd` - `COMMON` block with meteorological scalars
- `plhite.cmd` - `COMMON` block with plume heights for each source
- `segtab.cmd` - `COMMON` block with table entries for a particular segment

A.3 I/O Files

A list of the necessary Input Files with their standard names is given:

- Meteorological Initialisation File: `fort.41`
- First Meteorological Boundary File: `fort.41`
- Subsequent Meteorological Boundary Files: `fort.42`
- Concentration Initialisation File: `fort.41`
- Concentration Boundary File: `fort.41`
- File with Chemical Mechanism Input Parameters(automatically generated): `chemparm`
- File with Parameters to Control the Meteorological and Chemical Solver (manually provided): `bolchem.inp`

The following Output files are created:

- The Meteorological Output: `bolchem.mhf`
- The Concentration Output: `bolchem.chf`
- The Chemical Mechanism Control Field `simcontrol`

Appendix B

The Main Files of the Meteorological-Chemical Interface

B.1 bol2chem.f

```
      subroutine bol2chem(jstep)

#include "chparm.cmd"
#include "common.all"
#include "common.chem"
#include "bolcp.cmd"
        dimension p(NLON,NLAT,NLEV)
        ! avvezione
C        REAL conc1(NLON,NLAT,NLEV)
C       declaration added! (momme,14.11.2002 ) and cancelled
C       (momme,11.12.2002)
        real sundel(NLON,NLAT)
        real rough(NLON,NLAT)
c
C                                DATE
c
C CALCULATION OF SOLAR ELEVATION ANGLE, momme 10.12003
      IDAY =  INT(FLOAT(JSTEP)*DTSTEP/86400.)
      IHOU =  INT((JSTEP*DTSTEP-IDAY*86400.)/3600.)
      IMIN =  INT((JSTEP*DTSTEP-IDAY*86400.-IHOU*3600.)/60. +.5)
      IMIN  = IMIN + NMININ
      IF(IMIN.GE.60) THEN
      IMIN = IMIN - 60
      IHOU = IHOU + 1
      ENDIF
      IHOU  = IHOU + NHOUIN
        IF(IHOU.GE.24) THEN
        IHOU = IHOU -24
        IDAY = IDAY +1
        ENDIF
```

```
      IDAY  = IDAY + NDAYR
      dtmeteo=dtstep*ntgl/3600.
        do i=1,NLON
        do j=1,NLAT
C       roughness from bolam:
        rough(i,j) = brgm(i,j)
C       greenwich mean time:
        ltime = ihou*100 + imin
        call solarz(alatt(i,j),alont(i,j),0.,nyrin,1,iday,
     & ltime,sundel(i,j),5)
        do k=1,NLEV
C z-direction in chemical part and bolam inverted, momme 23.1.2003
        kinv=NLEV+1-k
C pressure calculation from bolam variables (momme. 9.1.2003):
         p(i,j,k)=ps(i,j)*sig(kinv)
        end do
        end do
        end do
        do l=1,NOSPEC

C         conc1(i,j,k)=conc(i,j,k,l)

C        call SL3DADV_chem(conc1)
        call SL3DADV_chem(conc(1,1,1,l))
C       direct passing more efficient, momme 11.12.2002
        end do

        ! chimica: sorgenti, diffusione verticale, reazioni
        call chemistry(conc,ctop,NLON,NLAT,NLEV,NOSPEC,
     .                                dtmeteo,U,V,P,T,PHIH,PHIG,
     .                 bustar,sundel,frvis,vegeta,rough,frdark,
     .                  rerr,aerr)

      return
      end
```

B.2 chemical.f

```
        subroutine chemistry(conc,ctop,nx,ny,nz,nspec,
     $                                dtmeteo,U,V,P,T,phih,phig,
     $                  ust,sundel,frd,veg,rough,fdark,
     $                  crerr,caerr)
C       changed name ustar to ust, ustar redundant to COMMON BLOCK!used?
C        implicit none
C        removed (momme:14.11.2002)
#include "chparm.cmd"
! CONTAINS CHEMISTRY PARAMETERS
#include "chdata.cmd"
! CONTAINS SPECIES INDICES, NAMES,
!   AND COEFFICIENTS
#include "cntrol.cmd"
! CONTAINS CONTROL PARAMETERS (added, momme
```

```
#include "mscal.cmd"
! CONTAINS CONTROL PARAMETERS (added, momme
C        14.11.2002)
        real T(nx,ny,nz),P(nx,ny,nz),U(nx,ny,nz),V(nx,ny,nz)
        real phih(nx,ny,nz),phig(nx,ny)
        real W(nz+1)
C  Declarations added, INITIALISATION?
        real sundel(nx,ny),frd(nx,ny)
        real db1(nx,ny)
        real db2(nx,ny)
C  qt not supported yet, momme 21.1.2003
C        real qt(nspec,nx,ny)
        real qt(nspec)
        real ctop(nspec,nx,ny)
C
        real conc(nx,ny,nz,nspec)
        real contem(nspec,nz)
        real dtmeteo
        real rough(nx,ny)
        real ust(nx,ny)
        real veg(nx,ny)
        real vd(nspec)
        real src(nspec)
        real flux(nspec)
        real windmg
C       dummy declarations of point source variables, momme 16.12.2002
        PARAMETER(npts=0,grav=9.807)
        real qpts(nspec,1)
        real ctest(nz+1)
        real a(nz)
        real b(nz)
        real c(nz)
        real y(nz)
        real x(nz)
        real tvert(nz)
        real th(nz)
        real xkz(nz+1)
        integer ijps(1)
        integer kpts(1)
        integer nzp
C       changed type of nzp (momme,14.11.2002)
C       z=1 surface layer, momme 23.1.2003
        kbeg=1
        nzp=nz+1
        frdark=fdark
        relerr=crerr
        abserr=caerr
C       point sources not supported, dump values
        ijps(1) = 1
        kpts(1) = 1
        DO l=1,nspec
        qpts(l,1) = 1.
        ENDDO
! compute the photolysis rates
```

```
        do i = 1, nx

           do j = 1, ny

            if(frd(i,j).lt.frdark)then
                ldark=.true.
            else
                ldark=.false.
            end if

               if (.not.ldark) then
                      call newphk (sundel(i,j))
               end if


                zlow=phig(i,j)

                do k = 1, nz
C z-direction in chemical part and bolam inverted, momme 23.1.2003
                       kinv = nz + 1 - k
C vertical vector of temperature for step3, momme (9.1.2003)
                tvert(kinv) = T(i,j,k)
C vertical cell thickness, momme 17.1.2003
                th(k) = phih(i,j,kinv)/grav - zlow
                zlow = phih(i,j,kinv)/grav

                  do l =1, nspec
                        contem(l,k) = conc(i,j,k,l)
C       qt not supported so far, momme 21.1.2003
                        qt(l) = 0.
                  end do

                end do ! loop on z

c           --CALCULATE GROUND LEVEL WIND SPEED FOR DIFCOF

            windmg =(sqrt(U(i,j,nz)*U(i,j,nz) + V(i,j,nz)*V(i,j,nz)))*3600
C calculate diffusion break, still to do!!!, momme 28.2.2003

        avdb = 0.
C            avdb  = (db1 (i,j) + db2 (i,j)) / 2.

C           --CALL DIFCOF TO GET USTAR
C                               DIFFUSIVITIES
C                               DIFFUSION RESISTANCE TO SINKS
C
C ustar passed from bolam, momme 22.1.2003
            ustar = ust(i,j)
            call difcof (nz, nzp, avdb, rough(i,j), windmg, th, xkz)

C           --CALL SNKSRC TO CALC SINK (VD) AND REEMISSION (SRC)
C
            if (.not.lsink) go to 150
```

```
            if (lterr) vegg = veg(i,j)
            call snksrc (vegg, difres,
     $               contem(1,kbeg), vd, src)
  150       continue

c           --call micro for surface-layer calcs
        tcll = T(i,j,nz)
        call micro (nspec, contem(1,kbeg),
     $          vd, src, qt(1),
     $          flux, contem(1,1), tcll,
     $          dtmeteo)

C           --CALL WINDZ TO CALCULATE OLD AND NEW VERTICAL WINDS
C
        call windz (nx, ny, nz, nzp,
     $        th,
     $        U, V, W,
     $        dtmeteo,
     $        contem, nspec)
C passing of time step added, momme 10.2.2003
C
C   vertical wind calculated and passed from bolam, momme 22.1.2003
C           --CALL STEP3 TO PERFORM VERTICAL ADVECTION

        call step3 (nz, nzp, nspec, npts, dtmeteo,
     $         th, xkz, W(1),
     $         contem,flux, ctop(1,i,j),
     $         ijps,kpts, qpts, tvert,
     $         ctest, A,
     $         B, C, Y,
     $         X)


! calculate the kinetic constants for each grid point and reaction
! involved
       do k=1,nz
C z-direction in chemical part and bolam inverted, momme 23.1.2003
               kinv = nz + 1 - k
               call newrk(T(i,j,kinv))

! if it is dark, calculate steady-state values of NO, NO2 and O3

!               if (ldark) then

!               call steady (contem(1,k))

!               end if

! call the chemical solver

               call step4 (contem(1,k),dtmeteo,T(i,j,kinv))

               do l =1, nspec
                      conc(i,j,k,l) = contem(l,k)
```

```
                end do

             end do ! loop on k

           end do ! loop on j

         end do  ! loop on i

         return

         end
```

B.3 iochf.f

```
C#########################################################################
      SUBROUTINE RDCHF(KUNIT,KFLAG)

C  READ CHF FROM KUNIT
C  KFLAG = 0 :  READ INITIAL CONDITION
C  KFLAG = 1 :  READ FIRST BOUNDARY CONDITION
C  KFLAG = 2 :  READ SUCCESSIVE BOUNDARY CONDITIONS

#include "chparm.cmd"
#include "common.all"
#include "common.chem"

      REAL concB1(NLON,NLAT,NLEV,NSMAX)
      REAL concB2(NLON,NLAT,NLEV,NSMAX)
C       addidional fiel declaration!
C  READ DESCRIPTOR RECORDS
C no input for calibration gas:
      nspec=nospec-1
      ICOUNT=0
 1    CONTINUE
C initial conditions
      IF(KFLAG.EQ.0) THEN
      READ(KUNIT,END=9001)
      READ(KUNIT)
      READ(KUNIT)
      ELSE
C boubdary conditions
      READ(KUNIT,END=9001)
      READ(KUNIT)
      READ(KUNIT)
      ENDIF


C  CHEMICAL SPECIES CONCENTRATION
      do ispec=1,nspec
      DO JLAT=1,NLAT
      DO JKLEV=1,NLEV
C initial conditions
      IF(KFLAG.EQ.0) READ(KUNIT)(conc(JLON,JLAT,JKLEV,ispec),
```

```
     .                                                          JLON=1,NLON)
C initial boundary condition
      IF(KFLAG.EQ.1) READ(KUNIT)(concB1(JLON,JLAT,JKLEV,ispec),
     .                                                          JLON=1,NLON)
C following boundary conditions
      IF(KFLAG.EQ.2) READ(KUNIT)(concB2(JLON,JLAT,JKLEV,ispec),
     .                                                          JLON=1,NLON)
      ENDDO
C read concentration fields on top of the region, momme 24.1.2003
      ENDDO
      end do
      do ispec=1,nspec
      DO JLAT=1,NLAT
      READ(KUNIT)(ctop(ispec,JLON,JLAT),JLON=1,NLON)
      ENDDO
        end do
C init calibration gas: momme. 5.3.2003
      DO JLON=1,NLON
      DO JLAT=1,NLAT
      DO JKLEV=1,NLEV
C initial conditions
      IF(KFLAG.EQ.0) conc(JLON,JLAT,JKLEV,nspec+1)=1.
C initial boundary condition
      IF(KFLAG.EQ.1) concB1(JLON,JLAT,JKLEV,nspec+1)=1.
C following boundary conditions
      IF(KFLAG.EQ.2) concB2(JLON,JLAT,JKLEV,nspec+1)=1.
C concentration on top of the region
      ctop(nspec+1,JLON,JLAT)=1.
      ENDDO
      ENDDO
      ENDDO
!      IF(KFLAG.EQ.0) THEN
!C  SURFACE CHARACTERISTICS     (to be implemented)
!      DO JLAT=1,NLAT
!      READ(KUNIT) (VEGETA(JLON,JLAT),JLON=1,NLON)
!      ENDDO
!      ENDIF

      WRITE(6,6001) KUNIT,KFLAG

      RETURN
 6001 FORMAT('   READ FILE FROM UNIT',I10,'     FLAG =',I10,/)
 9001 CALL SYSTEM('sleep 300')
      ICOUNT=ICOUNT+1
      IF(ICOUNT.GE.72) STOP !
      print*,' waiting....   icount=',icount
      GO TO 1
      END
C#########################################################################
      SUBROUTINE WRCHF(KUNIT)

C  WRITE CHF ON KUNIT
#include "chparm.cmd"
#include "common.all"
```

```
#include "common.chem"
      open(kunit,file='bolchem.chf',form='unformatted',status='unknown',
c     $     position='append')
     $iostat=ioend)
      rewind(kunit)
C no output for calibration gas:
      nspec=nospec-1
C  f77-standard doesn't include position option
c manual forward:
      DO
        READ(kunit,iostat=ioend)
        IF(ioend.NE.0) EXIT
      ENDDO
C     BACKSPACE(kunit)
C  WRITE DESCRIPTOR RECORDS

      WRITE(KUNIT) NFDR
      WRITE(KUNIT) NLSDR
      WRITE(KUNIT) PDR


C  CHEMICAL SPECIES CONCENTRATION
        do ispec=1,nspec
      DO JLAT=1,NLAT
      DO JKLEV=1,NLEV
       WRITE(KUNIT) (conc(JLON,JLAT,JKLEV,ispec),JLON=1,NLON)
      ENDDO
      ENDDO
        end do
      do ispec=1,nspec
      DO JLAT=1,NLAT
      WRITE(KUNIT)(ctop(ispec,JLON,JLAT),JLON=1,NLON)
      ENDDO
        end do
      WRITE(6,6001) KUNIT
      close(kunit)

      RETURN
 6001 FORMAT('   WRITTEN FILE ON UNIT',I10,/)
      END
```

B.4 wrhist.f

```
C#############################################################################
      SUBROUTINE WRHIST(KSTEP)

C  CHECKPOINT
C  KSTEP IS THE CURRENT TIME STEP
C  WRITE MHF AND CHF CONTAINING VARIABLES AT INSTANT KSTEP*DTSTEP (CHECKPOINT)
C  THE CHF FILE IS WRITTEN ON UNIT NUNHC

#include "common.all"
```

```
C  SDR AND PDR ARE UNCHANGED

C  DEFINITION OF FDR

      NFDR(1) = 1

C  DEFINITION OF VALIDITY DATE

      IDAY =  INT(FLOAT(KSTEP)*DTSTEP/86400.)
      IHOU =  INT((KSTEP*DTSTEP-IDAY*86400.)/3600.)
      IMIN =  INT((KSTEP*DTSTEP-IDAY*86400.-IHOU*3600.)/60. +.5)
        IF(IMIN.GE.60) THEN
        IMIN = IMIN - 60
        IHOU = IHOU + 1
        ELSE
        ENDIF
        IF(IHOU.GE.24) THEN
        IHOU = IHOU -24
        IDAY = IDAY +1
        ELSE
        ENDIF

      NFDR(7) = IDAY*10000+IHOU*100+IMIN

C  WRITE CHF ON UNIT NUNHI

      CALL WRMHF(NUNHI)
      CALL WRCHF(NUNHC)
C      if(kstep.gt.0) call wrrf(kstep)

      RETURN
      END
```

B.5 chread.f

```
      SUBROUTINE CHREAD(NCINP,NCTRC)
C
#include "chdata.cmd"
#include "chparm.cmd"
#include "cntrol.cmd"
#include "filcon.cmd"
#include "mscal.cmd"
#include "calib.cmd"
C
      LOGICAL LERROR
C*****************************************************************
      LERROR = .FALSE.
C
C     *** READ AND CHECK FILE DESCRIPTION HEADER RECORD
C
        nuchp = ncinp
        nutrc = nctrc
```

```
C input units passed from bolam, momme 28.1.2003
      OPEN(ncinp,file='chemparm',form='formatted',status='old')
      OPEN(nutrc,file='simcontrol',form='formatted',status='unknown')
      WRITE (NUTRC,2000)
C
      READ(NUCHP,1001)(NAM(I),I=1,10),(NID(J),J=1,60)
C
      WRITE(NUTRC,2001)NAM,NID
      DO 10 I = 1, 10
C         IF (NAM(I).EQ.NAMCHP(I)) GO TO 10
C         WRITE (NUTRC,1999) NAM, NAMCHP
C         STOP
 10   CONTINUE
C
      READ(NUCHP,1002)NOSPEC,NFAST,NSLOW,NRXN,NCOEFV,NCOC1,NCOC2,NPHOTK,
     &     NSC,NVTEMP, NVTCO, INDH2O
      WRITE(NUTRC,2002)NOSPEC,NFAST,NSLOW,NRXN,NCOEFV,NCOC1,NCOC2,
     &     NPHOTK, NSC,NVTEMP, NVTCO, INDH2O
C
      IF(NSC.GT.0) THEN
         READ(NUCHP,1013)(CKON(I),I=1,NSC)
         WRITE(NUTRC,2013)(CKON(I),I=1,NSC)
      ENDIF
C
C
C     *** READ SPECIES RECORD
C
      WRITE(NUTRC,2020)
      DO 20 I = 1, NOSPEC
         READ(NUCHP,1003)(MSPEC(J,I),J=1,10),LREAC(I),LSSIC(I),LSSBC(I),
     &        DVRES(I)
         WRITE(NUTRC,2003)(MSPEC(J,I),J=1,10),LREAC(I),LSSIC(I),LSSBC(I)
     &        ,DVRES(I)
 20   CONTINUE
C
C   ADD CALIBRATION GAS TO END OF LIST AND BUMP SPECIES COUNT
C
         NOSPEC = NOSPEC + 1
         KCLBR = NOSPEC
         DO 25 IND=1,10
            MSPEC(IND,KCLBR) = MCLBR(IND)
 25      CONTINUE
         LREAC(KCLBR) = .FALSE.
         LSSIC(KCLBR) = .FALSE.
         LSSBC(KCLBR) = .FALSE.
         DVRES(KCLBR) = 1.E10
C
C     *** TEST DIMENSIONS
C
      IF (NOSPEC.GT.NSMAX) GO TO 50
      IF (NRXN.GT.NRMAX) GO TO 50
      IF(NPHOTK.GT.NPHMAX) GO TO 50
      GO TO 100
C
```

```
C     *** DIMENSION ERROR
C
   50 WRITE (NUTRC,2050) NSMAX, NRMAX, NPHMAX
      LERROR = .TRUE.
      GO TO 800
C
C     READ LNITBAL TO SEE IF NITROGEN BALANCE WILL BE FORCED
C
 100  READ(NUCHP,1020)LNITBAL
C
      READ(NUCHP,1009)TREF
      WRITE(NUTRC,2009)TREF
C
C     READ THE ZENITH ANGLES FOR WHICH PHOTOLYSIS RATES ARE KNOWN
C
      READ(NUCHP,1010)NUMZEN,(ZENITH(II),II=1,NUMZEN)
      WRITE(NUTRC,2010)NUMZEN,(ZENITH(II),II=1,NUMZEN)
C
C     READ THE INDICES FOR PHOTOLYSIS RATE COEFFICIENTS
C
      READ(NUCHP,1011)(IPHRK(II),II=1,NPHOTK)
      WRITE(NUTRC,2011)(IPHRK(II),II=1,NPHOTK)
C
C     READ DUMMY LINES
C
      READ(NUCHP,'(//)')
C
C     ***  SET VARIOUS CONTROL FLAGS
C
C---ARE THERE ANY REACTIVE SPECIES
C
      NORS = 0
      LCHEM  = .FALSE.
      LANYSI = .FALSE.
      LANYSB = .FALSE.
C
C
      DO 150 L=1,NOSPEC
         IF (.NOT.LREAC(L)) GO TO 150
C
C        --REACTIVE--
C
         NORS = NORS + 1
         LCHEM = .TRUE.
         IF (LSSIC(L)) LANYSI = .TRUE.
         IF (LSSBC(L)) LANYSB = .TRUE.
C
  150    CONTINUE
C
C---IF THERE IS NO CHEMISTRY, THE ROADWAY FILE IS UNNECESSARY
C
      IF (.NOT.LCHEM) LRWY = .FALSE.
C
C---IF THIS IS A RESTART, DONT DO STEADY STATE ON INITIAL CONCS
```

```
C
      IF (LREST) LANYSI = .FALSE.
C
C     *** CALL SPECID TO IDENTIFY SPECIES
C
      CALL SPECID (NUTRC, NOSPEC, LREAC, MSPEC, ICOMP)
      IF (ICOMP.NE.0) LERROR = .TRUE.
C
C
C     ***  READ REACTION RECORD, IF ANY
C
  200 CONTINUE
C
      LANYPH = .FALSE.
C
      IF (NRXN.LE.0) GO TO 300
      NK=0
      WRITE(NUTRC,2004)
      DO 250 I = 1,NRXN
         READ(NUCHP,1004)RK(I), NRXTYP(I), NRXPAR(I)
         WRITE(NUTRC,2005)RK(I), NRXTYP(I),NRXPAR(I)
         IF(NRXPAR(I).GT.0)THEN
            IF(NRXTYP(I).EQ.7)THEN
               NK=NK+1
               LANYPH = .TRUE.
               READ(NUCHP,1005)(PHORAT(J,NK),J=1,NRXPAR(I))
            ELSE
               READ(NUCHP,1005)(RXNPAR(J,I),J=1,NRXPAR(I))
            ENDIF
         ENDIF
 250   CONTINUE
C
C     *** READ COEFFICIENTS RECORD, IF ANY
C
  300 CONTINUE
      READ(NUCHP,1006)(COEF(I),I=1,NCOEFV)
      READ(NUCHP,1006)(COEF(I),I=NCOC1,NCOC2)
      IF(NVTCO.GT.0)THEN
         READ(NUCHP,1012) (VTEMP(I),I=1,NVTEMP)
         READ (NUCHP,'(16I5)') (IVTCO(I),I=1,NVTCO)
         DO 310 I=1,NVTCO
            READ (NUCHP,'(6E13.6)') (VTCO(I,IT),IT=1,NVTEMP)
 310     CONTINUE
      ENDIF
C
C     *** CHECK FOR ERRORS
C
  800 IF (.NOT.LERROR) GO TO 9999
         WRITE (NUTRC,2700)
         STOP
C
 1001 FORMAT(10A1,60A1/)
 1002 FORMAT(/7(41X,I3/),5(41X,I2/))
 1003 FORMAT(/10A1,3L4,E14.4)
```

```
 1004 FORMAT(6X,E14.4,2I4)
 1005 FORMAT(11E12.4)
 1006 FORMAT(//(6E13.6))
 1009 FORMAT(/40X,F6.1)
 1010 FORMAT(//I5,11F6.1)
 1011 FORMAT(//20I4)
 1012 FORMAT(/(6E13.6))
 1013 FORMAT (16X,1PE14.6,18X,E14.6)
 1020 FORMAT(/42X,L1)
C
 1999 FORMAT (36H0***ERROR IN -CHREAD- *** FILE NAMED ,
     $  1OA1, 18H SHOULD HAVE BEEN , 10A1)
 2000 FORMAT (54H1****************  CHEMPARAM FILE  ******************)
 2001  FORMAT (32HOFILE DESCRIPTION HEADER RECORD /
     $  5X,17HFILE TYPE      = , 10A1 /
     $  5X,17HFILE ID        = , 60A1 /)
 2002  FORMAT (5X,36HNO OF SPECIES                    = , I3   /
     $  5X,36HNO OF FAST SPECIES               = , I3   /
     $  5X,36HNO OF SLOW SPECIES               = , I3   /
     $  5X,36HNO OF REACTIONS                  = , I3   /
     $  5X,36HNO OF VARIABLE COEFFICIENTS      = , I3 /
     $  5X,36HBEGIN OF CONSTANT COEFFS         = , I3 /
     $  5X,36HEND OF CONSTANT COEFFS           = , I3 /
     $  5X,36HNO OF PHOTOLYTIC REACTIONS       = , I2 /
     $  5X,36HNO OF CONSTANT SPECIES           = , I2   /
     $  5X,36HNO OF VARIABLE TEMPERATURES      = , I2 /
     $  5X,36HNO OF VARIABLE TEMPERATURE COEFFS = , I2 /
     $  5X,36HINDEX FOR CONCENTRATION OF H2O    = , I2 /)
 2003  FORMAT (5X, 10A1, 3L7, 1PE14.4)
 2004  FORMAT (/28HOREACTION PARAMETERS RECORDS //
     $ 7X, 2X, 10HRATE CONST,
     $     9X, 8HRXN TYPE, 6X, 17HNO OF PARAMETERS /)
 2005  FORMAT (6X, 1PE12.4, 2I16)
 2009 FORMAT (/5X,24HREFERENCE TEMPERATURE = , F7.2 /)
 2010 FORMAT (5X,26HNUMBER OF ZENITH ANGLES = , I5 /
     &     5X,12HANGLES ARE: , 11F6.1 /)
 2011 FORMAT(5X,44HCOEFFICIENT INDICES  FOR PHOTOLYSIS RATES : , / 5X,
     &     20I4 /)
 2013 FORMAT (/5X,33HCONSTANT SPECIES CONCENTRATION = ,1PE14.6)
 2020 FORMAT (/27HOSPECIES PARAMETERS RECORDS //
     $  5X, 10HSPEC NAME , 4X,5HREACT, 2X,5H SSIC, 2X,5H SSBC,
     $ 2X, 5HDVRES /)
 2050 FORMAT (31HOMAXIMUM DIMENSIONS EXCEEDED -- /
     $  9H SPECIES , I2/ 8H REACTS ,I3/ 19H PHOTOLYTIC REACTS , I2)
 2700 FORMAT (52HOPROGRAM TERMINATING IN -CHREAD- DUE TO ABOVE ERRORS)
C-----------------------------------------------------------------------
        CLOSE(ncinp)
        CLOSE(nutrc)
C
 9999 RETURN
      END
```

Appendix C

Exemplary Input Files

C.1 dimensioni_bolchem

```
      parameter (NLON=18, NLAT=18, NLEV=8)
```

C.2 bolchem.inp

```
&MODEL
NSTEP=100, DTSTEP=150., NHIST=1, NDRUNT=72, NLDIFF=.T., NLDDMP=.T.,
NBC=1, NTSBOU=1, NLVDFF=.T., NLDRYA=.T., NLSPONG=.T.,
NLSURF=.T., NLRAIN=.T., NLRAD=.T., NLCADJ=.T.,
NLANA=.T.,  NLMPG=.F., NLBPER=.F., NLBFIX=.T., NLEULR=.F.,
NADJ=4, NSTEPSL=6, HORDC=1.5, DIVDC=1.5,
NUNBC=41, NLRST=.F., NUNHC=30,NUNICC=31,NUNBCC=31,NCINP=29,NCTRC=28,
FRDARK=0., RERR=.1, AERR=1.E-03, NTGL=1
&END

           DEFAULTS FOR VARIABLES AND MEANING
               (ONLY FOR DOCUMENTATION)

NUNIC  = 41    (UNIT CONT. MET. INIT. COND. OR RESTART)
NUNHI  = 21    (UNIT TO WRITE MHF)
NUNBC  = 41    (UNIT CONT. THE FIRST MET. BOUND. FILE)
NUNDG  = 22    (UNIT TO WRITE MET. DIAGNOSTICS)
NUNRF  = 23    (UNIT TO WRITE MET. RESTART FILE)
NUNICC = 31    (UNIT CONT. INIT COND. OF CONC.)
NUNHC  = 30    (UNIT TO WRITE CONCENTRATIONS)
NUNBCC = 31    (UNIT CONT. THE FIRST CONC. BOUND. FILE)
NCINP  = 29    (UNIT INPUT WITH CHEMICAL MECHANISM)
NCTRC  = 28    (UNIT TO WRITE CHECKED CHEMICAL MECHANISM)
NADJ   = 4     (NUMBER OF ADJUSTMENT TIME STEPS)
NSTEP  = 1440  (TOTAL NUMBER OF TIME STEPS)
NSTEPSL= 10    (NUMBER OF TIME STEPS FOR EACH SEMILAGRANGIAN STEP)
DTSTEP = 60.   (TIME STEP IN S)
HORDC  = 1.    (SCALED HORIZONTAL DIFFUSION COEFFICIENT)
DIVDC  = 1.    (SCALED DIFFUSION COEFFICIENT OF DIVERGENCE)
NTSBOU = 0     (NUMBER OF TIME STEPS BETWEEN TWO BOUND. FILES)
NBC    = 1     (NUMBER OF AVAILABLE BOUNDARY FILES, INCL. INIT. COND.)
```

```
 NHIST  = 1440  (NUMBER OF TIME STEPS BETWEEN TWO CHEK POINTS)
 NDRUNT = 10    (  "       "    DIAGNOSTIC PRINTS ON STANDARD OUTPUT)

   NX1    = NLON/2 (COORDINATES DEFINING BOX FOR MPG DIAGNOSTICS)
   NX2    = NLON/2
   NY1    = NLAT/2
   NY2    = NLAT/2
   NZ1    = NLEV
   NZ2    = NLEV

1-  NLANA   = .FALSE.  (IF TRUE, ANALYSIS IS SAVED IN MHF AND PPF)
2-  NLBPER  = .FALSE.  (IF TRUE, PERIODIC B.C.)
3-  NLBFIX  = .FALSE.  (IF TRUE, FIXED B.C.)
4-  NLMPG   = .FALSE.  (IF TRUE, WRITES FILE MPG)
5-  NLDDMP  = .FALSE.  (IF TRUE, DIVERGENCE DAMPING ON)
6-  NLDIFF  = .TRUE.   (IF TRUE, HORIZONTAL DIFFUSION ON)
7-  NLDRYA  = .FALSE.  (IF TRUE, DRY ADIAB. READJ. ON)
8-  NLRAD   = .FALSE.  (IF TRUE, RADIATION AND SURFACE RAD. FLUXES ON)
9-  NLVDFF  = .FALSE.  (IF TRUE, VERTICAL DIFFUSION ON)
10- NLSURF  = .FALSE.  (IF TRUE, SURFACE THERMAL AND WATER BALANCE ON)
11- NLRAIN  = .FALSE.  (IF TRUE, LARGE SCALE RAIN ON)
12- NLCADJ  = .FALSE.  (IF TRUE, MOIST CONVECTIVE ADJ. ON)
13- NLEULR  = .FALSE.  (IF TRUE, EULERIAN ADVECTION OF HYDROMETEORS)
14- NLSPONG = .FALSE.  (IF TRUE, SPONGE LAYER SET NEAR THE TOP)
15- NLRST   = .FALSE.  (IF TRUE, RESTART)

  FRDARK  = 0. LOWER LIMIT FOR PHOTOLYTIC REACTIONS (W/M^2)
  RERR = .01 RELATIVE ERROR OF CHEMICAL SOLVER
  AERR = 1.E-06 ABSOLUTE ERROR OF CHEMICAL SOLVER
  NTGL = 1 CALL CHEMICAL SOVER EVERY NTGL STEPS OF BOLAM'S STEP
```

C.3 chemparm

```
CHEMPARAM      CHEMISTRY PARAMETERS     SARMAP.MOD
                SAPRC-90 MECHANISM FOR SARMAP MODEL (PRELIMINARY)

     NO OF SPECIES                     =  35
     NO OF FAST SPECIES                =  10
     NO OF SLOW SPECIES                =  25
     NO OF REACTIONS                   = 131
     NO OF VARIABLE COEFFICIENTS       = 163
     BEGIN OF CONSTANT COEFFS          = 451
     END OF CONSTANT COEFFS            = 467
     NO OF PHOTOLYTIC REACTIONS        = 16
     NO OF CONSTANT SPECIES            =  5
     NO OF VARIABLE TEMPERATURES       =  0
     NO OF VARIABLE TEMPERATURE COEFFS =  0
     INDEX FOR CONCENTRATION OF H2O    =  4

O2               2.090000E+05  M                1.000000E+06
HV               1.000000E+00  H2O              2.000000E+04
CH4              1.790000E+00
```

```
HNO3          T   F   F    0.1000E-09
HONO          T   F   F    0.2000E-02
HNO4          T   F   F    0.1000E+11
CO            T   F   F    0.1000E+11
HO2H          T   F   F    0.1000E+11
OOH           T   F   F    0.1000E+11
PAN           T   F   F    0.2940E-01
PPN           T   F   F    0.1000E+11
HCHO          T   F   F    0.1000E+11
CCHO          T   F   F    0.1000E+11
RCHO          T   F   F    0.1000E+11
MEK           T   F   F    0.1000E+11
RNO3          T   F   F    0.1000E+11
MGLY          T   F   F    0.1000E+11
AFG2          T   F   F    0.1000E+11
SO2           T   F   F    0.1000E+11
ETHE          T   F   F    0.1000E+11
OLE1          T   F   F    0.1000E+11
OLE2          T   F   F    0.1000E+11
OLE3          T   F   F    0.1000E+11
OLE4          T   F   F    0.1000E+11
ALK1          T   F   F    0.1000E+11
ALK2          T   F   F    0.1000E+11
ARO1          T   F   F    0.1000E+11
ARO2          T   F   F    0.1000E+11
O3            T   T   T    0.1470E-01
NO            T   F   F    0.2900E+00
```

```
NO2          T   F   F    0.1110E-01

NO3          T   F   F    0.2000E-02

N2O5         T   F   F    0.2000E-02

HO2          T   F   F    0.1000E+11

RO2          T   F   F    0.1000E+11

CCO3         T   F   F    0.1000E+11

C2CO3        T   F   F    0.1000E+11

CRES         T   F   F    0.1000E+11

LOGICAL VARIABLE FOR NITROGEN BALANCE IS: T

DEFAULT TEMPERATURE FOR REACTION RATES:  298.0

 ZENITH ANGLES
   11   0.0  10.0  20.0  30.0  40.0  50.0  60.0  70.0  78.0  86.0  90.0

 INDICES FOR PHOTOLYTIC REACTIONS
   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18  19

REACTION MECHANISM PARAMETERS

   1      0.0000E+00   7  11
  0.6779E+00  0.6738E+00  0.6587E+00  0.6342E+00  0.5918E+00  0.5244E+00  0.4023E+00  0.2368E+00  0.870
   2      0.2218E-04   4   3
  0.2155E-04  0.0000E+00 -0.4300E+01
   3      0.1436E+05   4   3
  0.9541E+04 -0.2380E+00 -0.1000E+01
   4      0.2328E+04   5   8
  0.3232E-02  0.0000E+00 -0.4000E+01  0.3229E+05  0.0000E+00 -0.1000E+01  0.6000E+00  0.1000E+01
   5      0.2694E+02   4   3
  0.2936E+04  0.2782E+01 -0.1000E+01
   6      0.4702E-01   4   3
  0.2055E+03  0.4968E+01 -0.1000E+01
   7      0.4155E+05   4   3
  0.2495E+05 -0.2980E+00 -0.1000E+01
   8      0.7073E-09   4   3
  0.1185E-09 -0.1050E+01 -0.2000E+01
   9      0.1868E+04   5   8
  0.7901E-01  0.0000E+00 -0.6300E+01  0.2202E+04  0.0000E+00 -0.1500E+01  0.6000E+00  0.1000E+01
  10      0.1747E-02   4   3
  0.3716E+14  0.2226E+02  0.1000E+01
  11      0.1478E-05   4   3
  0.1468E-05  0.0000E+00 -0.1000E+01
  12      0.5999E+00   4   3
  0.3670E+02  0.2440E+01 -0.1000E+01
  13      0.0000E+00   7  11
  0.1436E+01  0.1436E+01  0.1430E+01  0.1423E+01  0.1403E+01  0.1365E+01  0.1239E+01  0.1017E+01  0.676
```

```
14      0.0000E+00   7  11
0.1332E+02  0.1331E+02  0.1324E+02  0.1315E+02  0.1291E+02  0.1248E+02  0.1118E+02  0.8929E+01  0.5662
15      0.0000E+00   7  11
0.3745E-01  0.3737E-01  0.3697E-01  0.3641E-01  0.3536E-01  0.3370E-01  0.2978E-01  0.2379E-01  0.1565
16      0.0000E+00   7  11
0.2647E-02  0.2559E-02  0.2292E-02  0.1884E-02  0.1366E-02  0.8196E-03  0.3399E-03  0.7154E-04  0.6606
17      0.3251E+06   4   3
0.3229E+06  0.0000E+00 -0.1000E+01
18      0.4333E+05   4   3
0.2817E+05 -0.2510E+00 -0.1000E+01
19      0.7199E+04   5   8
0.2514E-01  0.0000E+00 -0.4600E+01  0.2202E+05  0.0000E+00 -0.1500E+01  0.6000E+00  0.1000E+01
20      0.0000E+00   7  11
0.1197E+00  0.1188E+00  0.1159E+00  0.1111E+00  0.1029E+00  0.8995E-01  0.6725E-01  0.3746E-01  0.1244
21      0.1698E+05   5   8
0.9337E-01  0.0000E+00 -0.5200E+01  0.3523E+05  0.0000E+00 -0.2300E+01  0.6000E+00  0.1000E+01
22      0.1551E+03   4   3
0.9468E+01 -0.1652E+01 -0.1000E+01
23      0.0000E+00   7  11
0.4083E-04  0.3981E-04  0.3669E-04  0.3178E-04  0.2513E-04  0.1735E-04  0.9099E-05  0.2927E-05  0.5047
24      0.3547E+03   4   3
0.3523E+03  0.0000E+00 -0.1000E+01
25      0.1005E+03   4   3
0.2349E+04  0.1870E+01 -0.1000E+01
26      0.1230E+05   4   3
0.5431E+04 -0.4800E+00 -0.1000E+01
27      0.2055E+04   5   8
0.6464E-02  0.0000E+00 -0.5200E+01  0.6899E+04  0.0000E+00 -0.2400E+01  0.6000E+00  0.1000E+01
28      0.2519E-02   4   3
0.1946E+14  0.2166E+02  0.1000E+01
29      0.6875E+04   4   3
0.1908E+04 -0.7550E+00 -0.1000E+01
30      0.3034E+01   4   3
0.1615E+02  0.9940E+00 -0.1000E+01
31      0.2595E+04   4   3
0.3229E+03 -0.1230E+01 -0.1000E+01
32      0.1862E-02   4   3
0.6823E-04 -0.1950E+01 -0.2000E+01
33      0.1443E+00   4   3
0.1113E-04 -0.5600E+01 -0.2000E+01
34      0.1036E+00   4   3
0.2370E-05 -0.6320E+01 -0.2000E+01
35      0.0000E+00   0   0
36      0.0000E+00   0   0
37      0.0000E+00   0   0
38      0.0000E+00   0   0
39      0.0000E+00   7  11
0.5267E-03  0.5189E-03  0.4938E-03  0.4531E-03  0.3921E-03  0.3098E-03  0.1989E-03  0.8736E-04  0.2169
40      0.2494E+04   4   3
0.4844E+04  0.3970E+00 -0.1000E+01
41      0.1471E+06   4   3
0.6752E+05 -0.4570E+00 -0.1000E+01
42      0.1140E+05   4   3
0.6165E+04 -0.3600E+00 -0.1000E+01
```

```
43      0.7365E+04   4   3
0.4991E+03 -0.1590E+01 -0.1000E+01
44      0.1478E+01   4   3
0.1468E+01  0.0000E+00 -0.1000E+01
45      0.1627E+05   4   3
0.2730E+04 -0.1053E+01 -0.1000E+01
46      0.0000E+00   0   0
47      0.0000E+00   0   0
48      0.0000E+00   0   0
49      0.0000E+00   0   0
50      0.0000E+00   0   0
51      0.0000E+00   0   0
52      0.0000E+00   0   0
53      0.0000E+00   0   0
54      0.0000E+00   0   0
55      0.0000E+00   0   0
56      0.0000E+00   0   0
57      0.0000E+00   0   0
58      0.0000E+00   0   0
59      0.0000E+00   0   0
60      0.0000E+00   0   0
61      0.0000E+00   0   0
62      0.1473E+05   4   3
0.7486E+04 -0.3970E+00 -0.1000E+01
63      0.1065E+05   5   8
0.7003E+01  0.0000E+00 -0.6000E+01  0.1233E+05  0.0000E+00 -0.1000E+01  0.2700E+00  0.1000E+01
64      0.7365E+04   4   3
0.4991E+03 -0.1590E+01 -0.1000E+01
65      0.2449E+05   4   3
0.4110E+04 -0.1053E+01 -0.1000E+01
66      0.2990E-01   5   8
0.9248E+14  0.2541E+02 -0.1000E+01  0.1320E+19  0.2670E+02  0.0000E+00  0.2700E+00  0.1000E+01
67      0.0000E+00   0   0
68      0.1241E+05   4   3
0.1233E+05  0.0000E+00 -0.1000E+01
69      0.0000E+00   0   0
70      0.0000E+00   0   0
71      0.0000E+00   0   0
72      0.2970E-01   4   3
0.9600E+19  0.2797E+02  0.0000E+00
73      0.0000E+00   7  11
0.2126E-02  0.2091E-02  0.1980E-02  0.1799E-02  0.1531E-02  0.1175E-02  0.7177E-03  0.2870E-03  0.6242
74      0.0000E+00   7  11
0.3070E-02  0.3036E-02  0.2923E-02  0.2737E-02  0.2441E-02  0.2011E-02  0.1367E-02  0.6465E-03  0.1721
75      0.1444E+05   4   3
0.1651E+04 -0.1288E+01  0.1000E+01
76      0.1167E+03   4   3
0.1424E+02 -0.1242E+01 -0.1000E+01
77      0.9060E+04   4   3
0.1440E+15  0.1391E+02  0.0000E+00
78      0.0000E+00   0   0
79      0.8910E+00   4   3
0.4110E+04  0.5000E+01 -0.1000E+01
80      0.2329E+05   4   3
```

```
 0.8147E+04 -0.6180E+00 -0.1000E+01
 81      0.0000E+00   7  11
 0.4160E-03  0.4062E-03  0.3758E-03  0.3277E-03  0.2615E-03  0.1824E-03  0.9651E-04  0.3088E-04  0.5129
 82      0.4029E+01   4   3
 0.2055E+04  0.3696E+01 -0.1000E+01
 83      0.2922E+05   4   3
 0.1248E+05 -0.5000E+00 -0.1000E+01
 84      0.0000E+00   7  11
 0.1496E-02  0.1465E-02  0.1369E-02  0.1216E-02  0.9991E-03  0.7294E-03  0.4148E-03  0.1502E-03  0.2957
 85      0.4029E+01   4   3
 0.2055E+04  0.3696E+01 -0.1000E+01
 86      0.1709E+04   4   3
 0.4286E+03 -0.8230E+00  0.1000E+01
 87      0.0000E+00   7  11
 0.1106E-03  0.1083E-03  0.1012E-03  0.8985E-04  0.7385E-04  0.5398E-04  0.3080E-04  0.1123E-04  0.2231
 88      0.3004E+04   4   3
 0.3216E+05  0.1408E+01 -0.1000E+01
 89      0.0000E+00   7  11
 0.5178E-03  0.5104E-03  0.4863E-03  0.4472E-03  0.3884E-03  0.3085E-03  0.1998E-03  0.8900E-04  0.2252
 90      0.2678E+04   4   3
 0.1732E+04 -0.2540E+00 -0.1000E+01
 91      0.5514E+04   4   3
 0.2628E+04 -0.4350E+00 -0.1000E+01
 92      0.0000E+00   7  11
 0.1183E-01  0.1178E-01  0.1161E-01  0.1133E-01  0.1083E-01  0.1000E-01  0.8269E-02  0.5651E-02  0.2712
 93      0.2542E+05   4   3
 0.2525E+05  0.0000E+00 -0.1000E+01
 94      0.0000E+00   0   0
 95      0.6207E+05   4   3
 0.6165E+05  0.0000E+00 -0.1000E+01
 96      0.3103E+05   4   3
 0.3083E+05  0.0000E+00 -0.1000E+01
 97      0.5256E+05   4   3
 0.1908E+05 -0.5960E+00 -0.1000E+01
 98      0.0000E+00   0   0
 99      0.6000E-01   4   3
 0.6000E-01  0.0000E+00  0.0000E+00
100      0.2542E+05   4   3
 0.2525E+05  0.0000E+00 -0.1000E+01
101      0.0000E+00   7  11
 0.3725E-01  0.3687E-01  0.3556E-01  0.3342E-01  0.2998E-01  0.2496E-01  0.1727E-01  0.8450E-02  0.2356
102      0.1313E+04   5   8
 0.1077E-01  0.0000E+00 -0.5300E+01  0.2202E+04  0.0000E+00 -0.1000E+01  0.6000E+00  0.1000E+01
103      0.3399E-01   4   3
 0.3376E-01  0.0000E+00 -0.1000E+01
104      0.1478E+03   4   3
 0.1468E+03  0.0000E+00 -0.1000E+01
105      0.3399E-01   4   3
 0.3376E-01  0.0000E+00 -0.1000E+01
106      0.1478E+03   4   3
 0.1468E+03  0.0000E+00 -0.1000E+01
107      0.1234E+02   4   3
 0.9182E+03  0.2548E+01  0.1000E+01
108      0.1259E+05   4   3
```

```
 0.2877E+04 -0.8700E+00 -0.1000E+01
109      0.2607E-02   4   3
 0.1761E+02  0.5226E+01 -0.1000E+01
110      0.1077E+04   4   3
 0.1527E+05  0.1574E+01 -0.1000E+01
111      0.2969E+00   4   3
 0.7971E+04  0.6043E+01 -0.1000E+01
112      0.4488E+05   4   3
 0.3083E+04 -0.1586E+01  0.0000E+00
113      0.1672E-01   4   3
 0.4245E+01  0.3279E+01  0.0000E+00
114      0.7232E+04   4   3
 0.6318E+04 -0.8000E-01  0.0000E+00
115      0.5194E+02   4   3
 0.1207E+04  0.1863E+01  0.0000E+00
116      0.9690E+05   4   3
 0.6712E+04 -0.1581E+01  0.0000E+00
117      0.2834E+00   4   3
 0.2968E+01  0.1391E+01  0.0000E+00
118      0.3824E+05   4   3
 0.1201E+05 -0.6860E+00  0.0000E+00
119      0.1538E+04   4   3
 0.1206E+04 -0.1440E+00  0.0000E+00
120      0.1481E+06   4   3
 0.1379E+05 -0.1406E+01  0.0000E+00
121      0.2110E-01   4   3
 0.6675E+01  0.3409E+01  0.0000E+00
122      0.8834E+05   4   3
 0.3256E+05 -0.5910E+00  0.0000E+00
123      0.9993E+03   4   3
 0.1645E+04  0.2950E+00  0.0000E+00
124      0.1648E+06   4   3
 0.4335E+05 -0.7910E+00  0.0000E+00
125      0.1888E+00   4   3
 0.1510E+00 -0.1320E+00  0.0000E+00
126      0.1002E+06   4   3
 0.3694E+05 -0.5910E+00  0.0000E+00
127      0.1267E+05   4   3
 0.3265E+04 -0.8030E+00  0.0000E+00
128      0.5318E+04   4   3
 0.3292E+04 -0.2840E+00  0.0000E+00
129      0.1512E+05   4   3
 0.7279E+04 -0.4330E+00  0.0000E+00
130      0.8669E+04   4   3
 0.8669E+04  0.0000E+00  0.0000E+00
131      0.4415E+05   4   3
 0.1627E+05 -0.5910E+00  0.0000E+00

VARIABLE COEFICIENTS
0.000000E+00 0.100000E-29 0.298000E+03 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.961360E+00 0.386440E-01 0.100000E+01 0.961360E+00 0.609680E+00
0.275140E+00 0.306140E-01 0.630610E-01 0.156960E+00 0.132320E+00 0.132320E+00
```

0.591450E+00 0.351910E+00 0.156890E+00 0.148800E+00 0.765350E-02 0.289260E+00
0.185000E+00 0.923470E-01 0.400000E+00 0.500000E+00 0.500000E+00 0.100000E+01
0.100000E+01 0.100000E+01 0.100000E+01 0.609680E+00 0.313790E+00 0.306140E-01
0.946430E+00 0.535750E-01 0.100000E+01 0.198230E+00 0.104900E+01 0.481900E+00
0.629330E-01 0.115790E+00 0.187700E+00 0.233910E+00 0.903200E-02 0.242940E+00
0.157240E-02 0.157240E-02 0.263580E+00 0.632800E+00 0.276030E+00 0.263210E+00
0.787110E-02 0.173500E+00 0.431460E-02 0.366730E-01 0.171750E+00 0.400000E+00
0.500000E+00 0.500000E+00 0.100000E+01 0.100000E+01 0.100000E+01 0.198230E+00
0.108590E+01 0.552060E+00 0.629330E-01 0.100000E+01 0.100000E+01 0.100000E+01
0.100000E+01 0.600000E-01 0.165000E+00 0.135000E+00 0.135000E+00 0.500000E+00
0.150000E+00 0.500000E+00 0.153000E+00 0.295000E+00 0.185000E+00 0.100000E+00
0.400000E+00 0.500000E+00 0.500000E+00 0.100000E+01 0.100000E+01 0.100000E+01
0.100000E+01 0.100000E+01 0.100000E+01 0.100000E+01 0.142230E+00 0.100000E+01
0.145780E+00 0.113530E+00 0.135000E+00 0.128670E+00 0.263670E+00 0.428880E-01
0.428880E-01 0.114000E+00 0.192890E+00 0.500000E+00 0.496110E+00 0.106290E+00
0.263130E-01 0.100000E+00 0.400000E+00 0.500000E+00 0.500000E+00 0.100000E+01
0.100000E+01 0.100000E+01 0.142230E+00 0.100000E+01 0.720280E+00 0.656180E-01
0.214100E+00 0.412450E+00 0.119840E+01 0.674070E-01 0.297960E+00 0.158560E+00
0.502920E+00 0.262980E-01 0.718420E+00 0.217310E+00 0.642660E-01 0.733200E+00
0.166890E+01 0.520040E-01 0.792420E-01 0.320050E+00 0.100020E+01 0.146450E-01
0.741310E+00 0.258690E+00 0.741310E+00 0.258690E+00 0.123820E+00 0.383950E+00
0.818830E+00 0.291080E-02 0.178260E+00 0.821740E+00 0.179720E+00 0.439840E+00
0.615150E+00

CONSTANT COEFICIENTS
0.200000E+01 0.500000E+00 0.150000E+01 0.155000E+00 0.105000E+01 0.480000E+00
0.160000E+00 0.139000E+01 0.150000E+00 0.750000E-01 0.850000E+00 0.200000E+00
0.220000E+00 0.156000E+01 0.370000E+00 0.440000E+00 0.120000E+00

Appendix D

The Makefiles

D.1 The BolChem Makefile

```
## paths
BASE            = $(HOME)/progetto/bolchem
SRC_PATH        = $(BASE)/src
CHEMSRC_PTH = $(SRC_PATH)/chemistry
INCLUDE_PATH = $(SRC_PATH)
RAD_PTH         = $(SRC_PATH)/radiation
BIN_LOCAL = $(HOME)/bin
## commands
SHELL =/bin/sh
RM =rm -f
FC =g77
LD =g77
## compiler and linker options
OPT1            = -x f77-cpp-input              # preprocessore
OPT2            = -Wall -ffortran-bounds-check  # controlli
OPT3            = -ffixed-line-length-none      # formattazione
# for CONFIG_OPTS see ./config_files/README
CONFIG_OPTS     = $(shell grep "extra_opts:" $(CONFIG) | cut -d':' -f2)
FFLAGS          = $(OPT1) $(OPT2) $(OPT3) $(CONFIG_OPTS)

INCLUDE         = -I$(INCLUDE_PATH)
FF_LIB          = -L$(CHEMSRC_PTH) -L$(RAD_PTH)
       # attenzione all'ordine delle librerie: il contrario non funziona
LIBS            = -lrad -lchem

## file names
CONFIG          ?= make.cfg
VERSION         = version.h
ENAME =  $(shell grep "exec_name:" $(CONFIG) | cut -d':' -f2 | tr -d ' ')
VNO = $(shell grep "version:" $(CONFIG) | cut -d ':' -f2 | tr -d ' ' | tr -d '\t')
EXEC = $(ENAME).v$(VNO)
SRC = bolam.f convec.f wrhist.f
OBJ             = $(SRC:.f=.o)
ARCHIVE         = libchem.a rad.a

## targets
```

```
all: $(EXEC)
echo $(VERSION)
#######################################################
# rules to make local library
$(ARCHIVE):
@echo '--------------------------------'
@echo 'Entering chemistry lib directory ...'
$(MAKE) -C $(CHEMSRC_PTH)
@echo '... leaving chemistry lib directory'
@echo 'Entering radaition directory ...'
$(MAKE) -C $(RAD_PTH)
@echo '... leaving radiation directory'
@echo '--------------------------------'
#######################################################


#######################################################
# creates (or updates) the version file, depending
# on the config file
$(VERSION): $(CONFIG)
@echo '--------------------------------'
@echo 'creating version.h ...'
echo -e "\tprint*,'...running BolChem v$(VNO) ...'" > $(VERSION)

@echo '... done'
@echo '--------------------------------'
#######################################################
#
#######################################################
# rules to build executable
$(EXEC): $(VERSION) $(OBJ) $(ARCHIVE)
$(LD) $(FF_LIB) $(OBJ) $(LIBS) -o $(EXEC)
@echo '--------------------------------'
@echo "`grep  "version:" $(CONFIG) | cut -d':' -f2`"
@echo 'executable $(EXEC) succesfully created'
@echo '--------------------------------'

#######################################################

#######################################################
# rules to make .o in the current directory (-c: don't link)
$(OBJ): %.o: %.f dimensioni_bolchem chemistry/chemparm
$(FC) $(FFLAGS) $(INCLUDE) -c $< -o $@
#######################################################


#######################################################
# rules to create/update dependencies
%.d: %.f
set -e; $(FC) $(INCLUDE) -M $(OPT1) $< \
| sed 's/\($*\)\.f\.o:/\1\.o $@:/g' > $@; \
[ -s $@ ] || rm -f $@

include $(SRC:.f=.d)
```

```
####################################################


####################################################
# rules for installing
install: $(EXEC)
mv $(EXEC) $(BASE)
ln -sf $(BASE)/$(EXEC) $(BIN_LOCAL)/bolchem
####################################################


####################################################
# rules for cleaning all
clean:
$(RM) $(OBJ) $(EXEC) $(SRC:.f=.d)
####################################################
```

D.2 The make-configuration File 'make.cfg'

```
version: 0.5.0
exec_name: BolChem
extra_opts: -g -fdebug-kludge -Wuninitialized
chem_xtra_opts: -g -fdebug-kludge -Wall
rad_xtra_opts: -r8 -g -fdebug-kludge -Wuninitialized
```

D.3 The Makefile for the Chemistry Library

```
INCLUDE_CPATH = $(HOME)/progetto/bolchem/src/chemistry
INCLUDE_PATH = $(HOME)/progetto/bolchem/src
AR = ar
ARFLAGS = crv
RM = rm -f

ARCHIVE = libchem.a
CONFIG ?= $(INCLUDE_PATH)/make.cfg
FC = g77
INCLUDE = -I$(INCLUDE_CPATH) -I$(INCLUDE_PATH)
OPT1    = -x f77-cpp-input
CONFIG_OPTS     = $(shell grep "chem_xtra_opts:" $(CONFIG) | cut -d':' -f2)
FFLAGS = $(OPT1) \
-Wall -ffortran-bounds-check \
-ffixed-line-length-none \
$(CONFIG_OPTS) \
$(INCLUDE)
SRC = $(shell ls RCS/*.f,v | cut -d, -f 1 | cut -d'/' -f 2 )
OBJ = $(SRC:.f=.o)

$(ARCHIVE): $(OBJ)
ar $(ARFLAGS) $(ARCHIVE) $?

####################################################
# rules to create/update dependencies
%.o: ../dimensioni_bolchem chemparm ../make.cfg
```

```
%.d: %.f
set -e; $(FC) $(INCLUDE) -M $(OPT1) $< \
| sed 's/\($*\)\.f\.o:/\1\.o $@:/g' > $@; \
[ -s $@ ] || rm -f $@
#
include $(SRC:.f=.d)
#####################################################

clean:
$(RM) $(OBJ:.o=.d) $(OBJ)
```

D.4 The Makefile for the Radiation Routine

```
INCLUDE_RPATH = $(HOME)/progetto/bolchem/src/radiation
INCLUDE_PATH = $(HOME)/progetto/bolchem/src
AR = ar
ARFLAGS = crv
RM = rm -f

ARCHIVE = librad.a
CONFIG ?= $(INCLUDE_PATH)/make.cfg
FC = fort77
INCLUDE = -I$(INCLUDE_RPATH) -I$(INCLUDE_PATH)
OPT1    = -cpp
CONFIG_OPTS     = $(shell grep "rad_xtra_opts:" $(CONFIG) | cut -d':' -f2)
FFLAGS = $(OPT1) \
-Wall -ffortran-bounds-check \
-ffixed-line-length-none \
-O3 \
$(CONFIG_OPTS) \
$(INCLUDE)
SRC = $(shell ls RCS/*.f,v | cut -d, -f 1 | cut -d'/' -f 2 )
OBJ = $(SRC:.f=.o)

$(ARCHIVE): $(OBJ)
ar $(ARFLAGS) $(ARCHIVE) $?

#####################################################
# rules to create/update dependencies


%.d: %.f
set -e; $(FC) $(INCLUDE) -M $(OPT1) $< \
| sed 's/\($*\)\.f\.o:/\1\.o $@:/g' > $@; \
[ -s $@ ] || rm -f $@
#
include $(SRC:.f=.d)
#####################################################

clean:
$(RM) $(OBJ:.o=.d) $(OBJ)
```

Appendix E

The *CHF* Format

A simple routine to create the *CHF* format:

```
        SUBROUTINE WCINIT(kunit)
C initialize concentration field
#include"chparm.cmd"
#include"common.all"
#include"common.chem"
        DO i=1,NLON
         DO j=1,NLAT
          DO n=1,NSMAX-1
           ctop(n,i,j)=1.
           IF (n.eq.1) ctop(1,i,j)=10.**6
           DO k=1,NLEV
           conc(i,j,k,n)=1.
           IF (n.eq.1) conc(i,j,k,n)=10.**6
           ENDDO
          ENDDO
         ENDDO
        ENDDO
C
        print*,'initialized chemistry!'
        print*,'writing...'
C
        WRITE(kunit) NFDRO
        WRITE(kunit) NLSDRO
        WRITE(kunit) PDRO
C
      do ispec=1,nsmax-1
      DO JLAT=1,NLAT
      DO JKLEV=1,NLEV
      WRITE(kunit)(conc(jlon,jlat,jklev,ispec),jlon=1,nlon)
      ENDDO
      ENDDO
      enddo
      do ispec=1,nsmax-1
      DO JLAT=1,NLAT
      WRITE(kunit)(ctop(ispec,jlon,jlat),jlon=1,nlon)
      ENDDO
       enddo
```

```
END
```

Bibliography

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[2] Liu M.K. et al. The chemistry, dispersion and transport of air pollutants emitted from fossil fuel power plants in california: Data analysis and emission impact model. Technical report, System Applications, Inc., San Rafael, CA, USA, 1976.

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