MULTI
Version 2.2 - August 1995

1 Introduction

This document is intended as a supplement to the documentation of MULTI version 1.0: *Carlsson, M.: 1986, Uppsala Astronomical Observatory Report 33: A Computer Program for Solving Multi-level Non-LTE Problems in Moving or Static Atmospheres.* The maintenance of a code for general use is very time-consuming and there are no resources for a full support in that respect for the code MULTI; the code is provided in the public domain and an attempt is made to incorporate bug-fixes in later versions but the use is entirely the responsibility of the user. The documentation is also patchy in its quality and it should only be regarded as an attempt to be of some help rather than a full-fledged support document.

Many persons have contributed with additions to the code. In particular I would like to thank Philip Judge, Martin Stift and Dan Kiselman for important contributions.

The version history is given in Section 2 with references to the sections where the options are described. A list of all INPUT variables is found in Section 18. Errata in earlier versions are covered in Section 17.

2 Version history

The main versions and changes implemented in them are (Section number for the description in paranthesis):

1.0
- Basic version described in Uppsala Report 33.

1.3
- Bug fixes in routines BMAT, FREQL, HSEINT (17)
- collisional/radiative switching (4)
- ISUM=0 (18)
- Fixed rates from given radiation field (5)
- Debye lowering of the ionization potential (16)
- Escape probability initial guess added (16)
- 20 character atomic energy level labels (16)
- DSCAL2 routine improved (16)
- GENCOL added (15)
- contribution functions calculated (16)
- easy conversion single-double precision (14)

2.0
- New opacity package (3)
- easier to incorporate new opacity data (3.1)
- background continua can be out of LTE (3.2)

- dimensioning upper bounds (6)
- local operator option (7)
- NG acceleration implemented (8)
- changed EMAX printout (16)
- common block alignment changed (9)
- character variables only stored in character data type (16)

2.2
- Incoming radiation field possible (10)
- Absorption profile may be linear combination of Voigt profiles (11)
- IDL adapted output routines (13)
- changed RINPUT (18)
- scattering in background opacity solved consistently (12)
- background opacity from lines can be added (3.3)

3 Background opacitites

A new opacity package is included based on the Uppsala package for calculating continous opacities (Gustafsson 1973). A minimum number of changes (mainly to include non-LTE effects) have been made to that package to facilitate a comparison with the original. The source code for the opacity package is rather opaque since it was originally written to minimize the use of core storage; a number of temporary files are used to that end. The input file specifying partition function data, photoionization cross-sections etc is called ABSDAT. This file is read in fixed format and when modified this has to be taken into account — do not change the format of the data!! For a detailed description of the data, see documentation in the source code. A condensed explanation follows.

3.1 Input file ABSDAT

The first line contains the number of elements to consider.
The second line contains the ID for the elements followed by the atomic weights for the elements.
The next line specifies how many ionization stages should be considered for the elements in the calculation of ionization equilibria. Only ionization stages included among the absorbers (further down) or important for the number of electrons need to be included.

A large block follows with data for the calculation of pressure and temperature sensitive partition functions followed by a table indicating which elements and which ionization stages to actually include (a series of lines with ones). NQFIX gives how many ionization stages should be calculated with fixed partition functions followed by lines with element index, ionization index and partition function value. NQTEMP gives the number of ionization stages to be treated with only temperature dependent partition functions. IFISH is a flag to indicate how to calculate an assymptotic part of the partition function.

TMOLIM gives a temperature above which no molecule equilibria will be calculated. A low value will switch off the calculation of molecules altogether while a standard value of

5000 will save some time without significantly affecting the equation of state. If molecules are the objective of the non-LTE calculation one should choose a high value to ensure molecule particle densitites to be calculated.

MOLH=0 gives calculation of all diatomic molecules involving H, C, N and O. MOLH=1 gives calculation of hydrogen molecules only.

After a block of coronal ionization data the opacity data follows. KOMP is the total number of opacity components included. Note the fixed format: do not move the numbers to the right or to the left.

For all the opacity components there is an ID of 20 characters (everything after character 20 will be treated as a comment) followed by a table with wavelengths and photoionization cross-sections (some normalized or in the form of Gaunt factors). This ID is used by MULTI to see if a background source is also included as a detailed photoionization cross-section in the MULTI atomic file. In order for this to work it is *essential* that the ID lines in ABSDAT and ATOM match exactly. Specifically this means that for hydrogen the labels have to be:
H BF N=1
H BF N=2
etc in both ABSDAT and ATOM. This is to make sure that the Lyman continuum opacity is not counted twice.

Photoionization cross-sections given after H^- and hydrogen are given level by level with the ID line starting with a slash (/). The line after the ID gives the ionization stage, the excitation potential in cm^{-1} and the statistical weight.

At the end there are tables of background opacities that are tabulated as functions of wavelength and temperature (the first one being H_{ff}).

3.2 How to get a background opacity in non-LTE

MULTI treats all background opacities as fixed and only one element at a time can be calculated. There is, however, a mechanism to iteratively get background opacities in non-LTE. This is regulated by the input variable IOPAC in the input file INPUT.

Setting IOPAC=4 causes the non-LTE solution of one element to be written to the unformatted file BMET2. Rename this file to BMET and run the next element with IOPAC=3. This causes the departure coefficient of the first element to be taken into account when calculating the background opacity from that element. The solution of both the first element and the second element are written to BMET2. Repeating for all elements of importance and iterating till convergence will give a consistent solution with background opacities in non-LTE. The values of IOPAC are thus:
IOPAC=2 BMET file is read. No file written.
IOPAC=3 BMET file is read. BMET2 is written with BMET merged with new solution
IOPAC=4 BMET2 file is written. No file read.

Again it is important that labels agree between ABSDAT and ATOM. Printout to the file OUT indicates which opacities that have been calculated in non-LTE.

3.3 Background opacity from lines

It is possible to include background opacity from lines by setting the input variable IOPACL>0 in the file INPUT. The input file with data for the lines is ABSLIN. The format of the file is:

Number of lines.

ID of line.
ID of lower level ionization stage
lower level ionization stage (1 is neutral), excitation energy (cm^{-1}), g-value
ID of uppwer level ionization stage
upper level ionization stage (1 is neutral), excitation energy (cm^{-1}), g-value
central wavelength, lower and upper wavelength when to consider line
f-value, damping constants for radiative damping, van der Waals and Starck.

Above block repeated for all lines. Wavelengths in Ångström and damping constants with same meaning as in the MULTI ATOM file.

Note that only elements calculated by the background opacity package can be included. One may have to add elements to ABSDAT or use an element with almost the same ionization potential and compensate differences in abundance by changing the f-value.

There is not yet an option to read in non-LTE populations for line opacities. It is possible to use a source function different from the Planck function by setting IOPACL=2. A two-level epsilon is calculated using the van-Regemorter formula for the collisional rate and setting the source function to (1-epsilon)*J + epsilon*B. IOPACL=1 gives the source function equal to the Planck function.

4 Collisional-radiative switching

The collisional-radiative switching technique of Hummer & S.A.Voels (1988) has been implemented. This technique is of very great help in cases where convergence is otherwise difficult to obtain due to very bad initial guesses and strong non-linearities, typically hydrogen. The option was eariler regulated by ICONV=2 and ICONV=3 but is now regulated by the INPUT variable ICRSW. The

ICRSW $= -2$ sets an automatic option. The first switching parameter is set to five times the maximum value of radiative rate over collisional rate and the collisional rates are multiplied by this value before iterations start. The value is then decreased by a factor of (1+FS0) per iteration. The starting value for FS0 is 9 such that the first decrease of the switching parameter is by a factor of 10. If lg(EMAX) goes over the value EREDO (set to 0.0) the iteration is redone with a smaller value of FS0. If EMAX is small, FS0 is increased. In most difficult cases this procedure leads to convergence albeit a large number of iterations may be needed.

ICRSW $= -1$ prompts interactively for values of the switching parameter. A negative value will cause the last iteration to be redone.

ICRSW > 0 causes the switching parameter to be decreased with ICRSW steps per decade in the log.

5 Transitions with given radiation field

Fixed rates calculated from a given radiation field and a given cross-section can be included. There are two major applications of this option

1. A photospheric radiation field from a calculation including line blanketing may be input and used to calculate photoionization rates.
2. The radiation field in one line may be calculated first (e.g. Lyman-β) and later be input as a pumping radiation field in another transition. Writing of the radiation field to file is set with INPUT variable IWJFIX.

The transitions with fixed radiation field are included as fixed transition in the ATOM file with ITRAD set to 4. Example input of a photoionization to be calculated with a fixed radiation field (taken from a 20-level + continuum model atom for lithium):

```
* FIXED TRANSITIONS
*   J  I IP     A0         TRAD   ITRAD
   21  1  1  1.416e-18     0.0       4
  21  1  1.416e-18    12   -1.0
     2299.500  1.41600e-18
     2249.500  1.44902e-18
     2201.500  1.47995e-18
     2155.600  1.50139e-18
     2069.300  1.53476e-18
     1989.600  1.56107e-18
     1915.800  1.56986e-18
     1847.300  1.57645e-18
     1783.500  1.56785e-18
     1724.000  1.55685e-18
     1668.300  1.54629e-18
     1616.100  1.52859e-18
```

Note that after the line giving IP=1 and ITRAD=4 follows specification of the photoionization cross-section in the same format as for a bound-free transition treated in detail. The same is true for a bound-bound transition with a given radiation field (example from an atomic model of oxygen where there is pumping from Lyman-β):

```
* FIXED TRANSITIONS
*   J  I IP     A0         TRAD   ITRAD
   13  1  0  2.022E-02     0.0       4
*  J  I     F        NQ   QMAX  Q0 IO     GA         GW          GQ
  13  1  2.022E-02 25   50.0  4.0 0  9.598E+07 1.000E+00 5.943E-06
```

The fixed ratiation field is read from file JFIX. The file is unformatted and direct access with a record length in words equal to the number of depth-points for the JFIX data. The file contains:

1. A header record with the number of frequencies and depth points.
2. Record/records with frequencies in Hz.
3. Record with $\lg \tau_{5000}$.
4. Record with $\lg m_c$ where m_c is the column mass.
5. Records with $\ln J_\nu/B_\nu$ as a function of depth, one record for each frequency.

Note that the JFIX data are interpolated in frequency to the frequencies in the line or bound-free transition that is to be treated with a fixed radiation field. This means that it is not meaningful with a much denser frequency grid in JFIX than in the atomic transitions affected. Line-blanketing mean intensities should then be smoothed to the typical spacing in the photo-ionization data before written to JFIX. Note also that it is the natural logarithm of the ratio between the mean intensity and the Planck function that should be in the JFIX file.

If the depth-grid in MULTI extends past the depth-grid in the JFIX file extrapolation is performed. At the top the topmost value of J_ν from the JFIX file is used. At the bottom extrapolation causes J_ν to be set to the Planck function.

The routine JFIX is unformatted. If it has been written in double precision it has to be read in double precision as well. When moving from one machine platform to another it may be necessary to convert the format of the JFIX file.

6 Dimensioning of code

The matrix W and array E are passed as arguments instead of through a common block. This has made it possible to implement MK1 and MDEP1 as upper bounds instead of exact limits (as was the case in version 1.3). The PARAMW include file has been kept with MK1 and MDEP1 as separate parameters (instead of using only MK and MDEP) in order to save recompilation and memory. The main memory usage is still in matrix W and this can be kept to a minimum through setting MK1 and MDEP1 to rather low values with MK and MDEP higher. Changing MK1 and MDEP1 will only cause recompilation of the main program.

7 Local operator

A local approximate lambda operator option has been implemented (Olson et al. 1986, see also Puls & Herrero 1988). The local operator is very much less memory demanding which makes it possible to solve problems with very large model atoms (more than 100 levels).

The distribution includes both the old global operator and the local operator options - only a few subroutines differ. Both operators have their advantages, see Carlsson (1991) for a discussion.

8 Convergence acceleration

Ng acceleration is implemented (Auer 1987). This will cause faster convergence, especially with the local operator version. Ng acceleration is switched on by setting the INPUT variable INGACC to a non-zero value. The default is INGACC=1. (In Multi 2.0 Ng-acceleration was switched off by adding 10 to the value of ICONV — ICONV=10 corresponded to ICONV=0 but with NG acceleration switched off etc. ICONV values larger than one are no longer allowed since this functionality has been transfered to the variable INGACC).

9 Common block alignment

Common block alignment was a problem with the old version and some RISC architectures. This has been fixed by separating variables of different type into separate common blocks in the include files. The include file CATOM thus contains common blocks CATOMI for integer type variables and CATOM for floating point variables. It is recommended that modifications of the code stick to this convention.

10 Incident radiation field

It is possible to read in an incident radiation field from file. The option is switched on with INPUT variable INCRAD. The incident radiation field will then be read from formatted file IMINUS that contains

SCALEI	global scaling factor
NMUI	number of angle points
NXL	number of wavelength points
XL(q) I^{-}(q,1)...I^{-}(q,NMUI)	wavelength in Ångström, I^{-}, wavelength point q
...	

Only NMUI=1 with I^{-} independent of μ has been implemented. Only bound-free (photoionization) transitions are considered. "Exact" match between wavelengths given in the file IMINUS and for the photoionization data in the file ATOM is needed for I^{-} to be set. This is because I^{-} for many applications consist of coronal radiation in discrete lines integrated over wavelength bins. It is then necessary to remap the bins to the wavelength bins used for the transition.

11 Blends and multiplets

There is no consistent provision for blends in MULTI version 2.3. One of the most common applications is the calculation of multiplets where the components overlap but where the close upper or lowere levels can be assumed to be populated with relative populations proportional to the statistical weights of the levels. This case can now be handled by treating the multiplet as a single transition and the terms as conglomerate levels with the atomic absorption profile set to a linear combination of profiles of the involved detailed transitions. This is best illustrated with an example. In neutral lithium the resonance line is a doublet with lower level $1s^2\,2s\,^2S_{1/2}$ and upper levels $1s^2\,2p\,^2P^o_{1/2}$ and $1s^2\,2p\,^2P^o_{3/2}$. The upper level energies are 14903.66 and 14904.00 cm^{-1} with statistical weights 2 and 4 respectively. The lines have f-values of 0.251 and 0.502. To treat this doublet as a single line, the upper levels are merged into one with an energy equal to the weighted average of the two resulting in 14903.89. The statistical weight will be 6 (the sum of the two) and the f-value of the term transition with common lower level is the sum of the two, 0.753. In the ATOM file we give the conglomerate transition with the IWIDE variable IO set to 2 to signal that the profile function should be calculated as a linear combination of 2 profiles (IO=3 signals 3 components etc). Data for the components follow with
ΔE (in cm^{-1}), weight of component in weighted average, f-value, GA, GW, GQ
the energy difference for a component transition is the term energy difference plus the ΔE given above. For the lithium example the lines necessary in ATOM are:

```
* UP LO      F          NQ   QMAX   Q0 IO       GA           GVW        GS
   2  1  7.530e-01     59   20.0  2.0  2  3.719e+07        1.0  0.000e+00
    -0.227  0.3333  2.510e-01               3.719e+07        1.0  0.000e+00
     0.113  0.6666  5.020e-01               3.719e+07        1.0  0.000e+00
```

12 Scattering in the Background Source Function

The background source function is in general a linear combination of an absorption part and a scattering part:

$$S_c = \sigma_c/\chi_c J_\nu + \kappa_c/\chi_c B_\nu$$

where σ_c is the background scattering, χ_c is the background opacity and κ_c the background absorption. In earlier versions the scattering part of the background source function was lambda iterated: J_ν in the above formula was set to the value from the previous iteration. When scattering dominates the background source function and the line source function is small this sometimes lead to slow convergence or even stabilization. A new routine has now been incorporated, TRANSC, which solves the transfer equation with scattering treated self-consistently at the expense of more computing time. This routine is used if INPUT variable ISCAT=1. It is also used when calculating the radiation field from a restart (ISTART=-1) and when calculating LTE equivalent widths. The lambda iterations previously used gave printouts of the type:

```
LOG(LTEEQW SCAT EMAXJ)=    0.0000  LTEEQW SCAT EMAXJ= 1.0000E+00
LOG(INITIA SCAT EMAXJ)=    0.0000  INITIA SCAT EMAXJ= 1.0000E+00
```

These printouts do not occur anymore.

13 IDL output

The old output routines have been complemented with routines that write data to unformatted files to be processed with IDL (Interactive Data Language). This makes it possible to interactively and graphically study all variables. IDL procedures to read the data and perform some of the processing are provided in the MULTI distribution. The writing of the IDL files is now governed by INPUT variables IDL1, IDLNY and IDLCNT (in earlier versions this was accomplished by setting existing INPUT variables to strange values). The file always needed is IDL1; it contains most variables. With IDL1=1 it is written in default format containing a lot of data. For very large model atoms and grids of runs one may run out of diskspace. For such a case there is another format that can be chosen with IDL1=2. Indices for lines of interest are read from file KRSEL and only data for those lines are written to the IDL1 file. Some large arrays, like the collisional rates C(I,J,K) are not written. The variables that are frequency dependent but not stored for all frequencies in MULTI (like TAUQ, X, S) are written to the IDLNY file. This file can become very large. Contribution functions are written to IDLCNT, opacities to IDLOPC (governed by INPUT variable IWOPAC).

14 Double precision

The code has been modified in order to make a transition to a double precision version very simple. Slight modifications have been made in most routines:

- all specific intrinsic function names have been changed to generic (ALOG has been changed to LOG etc).
- REAL constants in subprogram argument lists have been changed to REAL type variables.
- DIMENSION is used instead of REAL in declarations.
- REAL type local variables starting with letters I-N have been renamed so they start with letters A-H or O-Z (with the exception of the opacity package).
- A statement INCLUDE 'PREC' has been added to all routines.

In order to make a double precision version, the following steps should be carried out:

1. the PREC include file should contain the statement
   IMPLICIT REAL*8 (A-H,O-Z)
   or the equivalent FORTRAN-77 extension in the local FORTRAN dialect.
2. REAL should be replaced with REAL*8 in all include files (COMMON-blocks).
3. REAL should be replaced with REAL*8 in the opacity package and the routine OPAC.
4. the record length of direct access files in routine OPEN should be doubled (RECL=IRECW*2 instead of RECL=IRECW).

15 General collisional routine

In version 1.0 the user was assumed to write his own collisional routine for every element he was interested in. From version 1.3 this is no longer necessary; there is a routine GENCOL that accepts collisional data in a variety of formats. See comments in that routine for details.

16 Other code changes

Debye lowering of the ionization potential is taken into account when calculating LTE populations

An escape probability solution has been added as an option for the initial guess.

Some changes to the printout formats have been made.

Atomic energy level labels may have up to 20 characters instead of only 4.

Ionization ratio changes and column mass changes are taken into account in the routine DSCAL2 when calculating a new depth-scale. The depth-scale written to file DSCAL2 will thus be useful also in hydrogen runs.

Contribution functions are calculated and printed.

17 Errata

17.1 ERRATA MULTI version 1.3 corrected 20-APR-1994

An error in the routine QCALC affected the total poppulation densities of the energy levels treated in detail when solving the non-LTE problem for molecules CO, CH or CN. The populations were a factor of four too small. Note that this error only affected the non-LTE solution for any of these molecules and not the density of molecules calculated by the background opacity package.

17.2 ERRATA MULTI version 1.3 corrected 08-JUN-1989

There are two errors in the radiative-collisional switching coding in version 1.3 of MULTI. The errors will only affect runs with hydrogen where hydrostatic equilibrium integrations are performed. Both errors are in the routine ITER.

The first error is that HSEINT is called as soon as EMAX is less than ELIM1 even if the switching parameter SWITCH is larger than one. This will cause unnessesary work. When the maximum correction to the electron densities in HSEINT (CORMAX) is less than ELIM2 there will be no more hydrostatic equilibrium integrations. In the unlikely event that SWITCH is larger than one the final hse integration will not be consistent with the non-LTE solution.

The cause of the second (really important) error is that the total fixed rates stored in C(I,J,K) are calculated from the atomic collisional rates multiplied by the switching parameter SWITCH plus the fixed rates. This is done by reading the collisional rates from the file DUMC and storing them in the variable COL and storing the fixed rates C-COL in variable FIX. This is however done *outside* the iteration loop. After a hydrostatic equilibrium integration there are new electron densities and therefore new collisional rates. These new rates are overwritten by the old rates calculated from COL*SWITCH+FIX. The effect is that the collisional rates will always be calculated from the electron densities in the original atmosphere and not from the current electron densities from the last hydrostatic equilibrium calculation.

A check to see if any of these errors have affected the results is to make a run using the output atmosphere (ATHSE file) as input atmosphere (ATMOS file). There should be no significant changes in such a run.

17.3 ERRATA MULTI version 1.3 corrected 16-FEB-1988

There are some errors in the routines BMAT, FREQL and HSEINT in Uppsala Observatory Report 33.

BMAT (page Appendix A 20)

There is an error in the boundary condition. If the optical depth at any frequency-angle at the first depth-point is so large (on the order of 10) so the diffusion approximation is to be used, that is not possible in the first depth-point. If the optical depth is larger than 20, the intensity is set equal to the source function. If the optical depth is less than 20, an expression taken from the boundary condition in the transfer solver is used. This expression is erroneous in the Uppsala report. The error may affect the convergence (even causing divergence or stabilization with corrections around one percent never getting any smaller) but does not affect the solution in a converged run (since the error is in the approximate matrix and not in the formal solver). If lines are optically thin at the topmost depth-point, the error will not show up.

FREQL (pages Appendix A 35-36)

Added options gave incorrect weights for IND = 1. This affected cooling rates for lines with frequency quadrature given with QMAX = $Q0$ or QMAX $<$ 0 or Q0 $<$ 0. The corrected weights are twice the old ones.

HSEINT (pages Appendix A 58-60)

1. Wrong units for VTURB in formula for turbulent pressure.
2. Wrong expression for turbulent pressure.
3. Slight error in the derivative in the Newton-Raphson scheme of typically a factor of 1.1.
4. Hydrogen populations taken from radiative transfer and not from hydrostatic equilibrium in the first N-R iteration. This might lead to errors if the correction in the first iteration is smaller than 1.E-4.

The two first errors only matter if turbulent pressure is important, error 3 only affects the rate of convergence and not the solution. Errors 3 and 4 have been carried over from the Uppsala version of LINEAR-B that was the model for the HSEINT routine and might be present in other versions of the code LINEAR as well.

None of the errors is significant for a solar atmosphere and if hydrostatic equilibrium iterations are not performed, HSEINT is never called.

18 INPUT variables

The routine RINPUT has been rewritten now allowing for default values for variables missing in the INPUT file. A number of new INPUT variables has been introduced to switch on and off new features. Some of these new features were regulated by old INPUT variables in versions between 1.0 and 2.2. Ng acceleration was switched off by adding 10 to the value of ICONV; this is now handled by setting the INPUT variable INGACC=0. Some of the IDL output was switched on by setting IW variables to negative values. All in all very difficult to remember. The reason was to keep backward compatability with old INPUT files (tons of them exist). This is now done by setting default values to all new INPUT variables.

The full list of INPUT variables with explanations are:

DIFF — Diffusion parameter. When $\Delta\tau_{\nu\mu}$ is larger than DIFF the diffusion approximation is used in routine BMAT. A value of 5 has normally been used without causing problems.

ELIM1 — When the maximum relative correction in the population numbers, EMAX, decreases below this value, the matrix W is not recalculated and only back-substitutions are performed in EQSYST. This saves a lot of computing time but the value has to be sufficiently small so that the matrix is not too far from the correct one. A value of 0.1 has been proven safe.

ELIM2 — When EMAX decreases below this value the iteration procedure is stopped and the populations are then used in the formal solution. The difference between the populations and the infinitely converged populations is normally a factor 5–10 smaller than EMAX. The value chosen depends on the internal accuracy wanted. A value smaller than 0.01 is seldom neither needed nor meaningful since other errors (basic assumptions, depth discretization etc) are larger.

QNORM — All relative frequencies in the program are in a unit determined by a scaling constant, the value of which is given by QNORM. The unit of QNORM is km per second at line center. The value is arbitrary and a change of QNORM results in a scaling of all the frequencies. It is recommended to set QNORM to a typical Doppler width in km per second at line center. It is then easier to specify the frequency quadrature, to locate the transition from the Doppler core to the wings in strong lines etc.

THIN — When $\tau_{\nu\mu}$ is less than THIN the radiation field is in effect lambda iterated. This improves the stability properties and reduces the CPU time required for each iteration, see Section 3.2 in the Uppsala report. A value of 0.1 has been optimal in almost all cases studied.

IATOM2 — It is possible to go through the formal solution with a new set of atomic levels or transitions read from the file ATOM2. The converged populations are then redistributed to the new levels that have the same label as the old ones. This is done proportional to the statistical weights. The file ATOM2 is only read if IATOM2=1. This option can be used such that the file ATOM contains the terms and conglomerate lines while ATOM2 contains the explicit sublevels and lines and/or other frequency points.

ICONV The populations and the ionization fractions are always written to the file OUT (if IWN$\neq$0). The rest of the printout will depend on the value of ICONV. If ICONV=0 only a converged solution will give detailed printout, If ICONV=1 a detailed printout will always be attempted. Normally ICONV is set to 0 to avoid time consuming nonsense printouts and possible arithmetic overflows from a non-converged run. In some instances this printout is of interest even if EMAX is greater than ELIM2; notably when ITMAX=0. ICONV=1 will then force these detailed printouts.

IHSE Used only if the model atom is hydrogen. The value then determines if hydrostatic equilibrium (HSE) integrations should be performed.

ILAMBD Determines the number of lambda iterations to be performed on the starting approximation determined by ISTART. A value larger than 1 is hardly needed.

IOPAC When a restart is done with no changes influencing the background opacities it is not necessary to recompute these. IOPAC=0 will read the file INIT and use the old opacity file OPC. The normal value is IOPAC=1. For background opacities in non-LTE values of 2, 3 and 4 are used. IOPAC=4 writes the file BMET2, IOPAC=2 reads the file BMET, IOPAC=3 reads BMET and writes BMET2, see section 3.2.

ISTART Determines the starting approximation together with ILAMBD. ISTART=0 sets the intensities equal to zero in the rates and then solves the statistical equilibrium equations. ISTART=1 sets the populations equal to the LTE values. ISTART=-1 reads the starting approximation from the file RSTRT; for the format see routine WRSTRT. Such a file is written by the routine WRSTRT at the end of each run and this file can then be used for a restart or to get additional printouts without running the whole problem anew. For the latter application set ITMAX=0 and ICONV=1. ISTART $>$ 1 uses an escape probability starting solution with ISTART-1 iterations from $n = n^{LTE}$

ISUM The statistical equilibrium equation for level ISUM is replaced by the particle conservation equation. If the statistical equilibrium equation for one level has much smaller coefficients than the others it should NOT be replaced. This is often the case for the continuum level. If ISUM=0 the code will choose the level with the highest population density to be replaced - normally a safe option. If numerical instabilities seem to be present a good first try is to change the value of ISUM.

ITMAX The maximum number of iterations allowed. Most cases studied converge in 3–8 iterations, hydrogen with HSE integrations requires more, 10–20. Using a local operator also gives slower convergence. With collisional-radiative switching a very large value is needed, 50–100. If the populations seem to converge but ITMAX iterations were insufficient to meet the ELIM2 criterion it is possible to continue from the partially converged solution, see variable ISTART. A value of 0 makes it possible to do only the formal solution for known populations, see variable ICONV.

ITRAN Determines the method of solving the equations of radiative transfer with a known source function. ITRAN=0 gives the ordinary Feautrier method, ITRAN=1 gives the Feautrier method with cubic spline accuracy, ITRAN=2 gives the Feautrier method with Hermite accuracy. On a depth scale smooth in max $\Delta \lg \tau_{mu\mu}$ ITRAN=2 will give a higher accuracy but if the depth scale is very irregular instabilities may occur, see Section 3.3 in the Uppsala report. ITRAN=3 (not recommended) and ITRAN=4 gives an integral method based on fitting the source function with a cubic spline, see routine TRANI.

NMU Gives the number of angle points to be used. Normally it is sufficient with three points in static atmospheres and five in atmospheres with velocity fields.

IWxxxx Printout option. IWxxxx=0 inhibits printout from the specific routine. IWxxxx>0 normally gives a printout for every IWxxxx depth point. If IDL is available, most printouts should be switched off and the IDL routines used instead (see variables IDL1, IDLNY and IDLCNT).

IWABND Abundances printed to file OUT.

IWATMS Atmospheric parameters printed to file OUT.

IWATOM Atomic parameters printed to file OUT.

IWCHAN Graphic convergence pattern printed to file OUT. Seldom of interest and quite large.

IWDAMP Damping parameters printed to file OUT.

IWEMAX Maximum corrections to population densities and to mean intensities printed to file OUT and to the standard output (terminal). Very useful.

IWEQW Equivalent widths printed to file OUT.

IWEVEC Error vector printed to file OUT. Only of debugging interest and very voluminous.

IWHEAD Heading lines printed to file OUT. Useful.

IWHSE Hydrostatic equilibrium printout to file OUT.

IWLGMX Maximum steps in max $\Delta \lg \tau_{mu\mu}$ printed to file OUT. Very useful in checking depth-scale.

IWLINE Transition data written to file OUT.

IWLTE LTE populations written to file OUT.

IWN Populations and ionization fractions written to file OUT.

IWNIIT Populations as function of depth and iteration written to file NIIT.

IWOPAC Opacities written to files OUT and IDLOPC.

IWRAD Radiation quantities written to file OUT.

IWRATE Rates written to file OUT. Difficult to interprete and lots of data.

IWSTRT Starting approximation written to file OUT.

IWTAUQ Monochromatic optical depths written to file OUT. Lots of data.

IWTEST Lots of debug-character data written to file OUT.

IWWMAT Matrix written to file WMAT.

IWJFIX File JFIX2 written. Switched on by IWRAD < 0 in earlier versions.

IWARN Warning messages can be partly switched off with IWARN. A value of zero switches off all but the most important warning messages, IWARN=1 includes more warning messages but excludes warnings about negative opacities (these warnings are seldom of any consequence and can fill up the JOBLOG file). Default value is IWARN=2.

IOPACL Regulates the inclusion of background opacities from lines. IOPACL=1 sets the source function to the Planck-function for background lines; IOPACL=2 uses a two level formula with the collisional rate calculated with the van Regemorter formula. See section 3.3. Default value is IOPACL=0.

ISCAT ISCAT=1 switches on a scattering version of Feautrier solving consistently for the scattering part of the background source function. If there is a lot of scattering in the continuum opacity the standard lambda iteration of the background source function may lead to slow convergence (or even stabilization). ISCAT=1 solves this problem at the expense of more computing time. Default value is ISCAT=0.

INCRAD INCRAD=1 flags the inclusion of an incident radiation field. This radiation field is read from the file IMINUS. See section 10. Default value is INCRAD=0.

INGACC INGACC=1 flags the application of Ng acceleration to the iteration procedure. Almost necessary in connection with the local operator and often useful also for the global operator. Will sometimes lead to divergence. Default value is INGACC=1.

ICRSW ICRSW=–2 will switch on collisional-radiative switching (see section 4 with values determined automatically.
ICRSW=–1 will prompt reading of values interactively.
ICRSW > 0 will decrease the switching parameter equidistantly in the log with ICRSW steps per decade.
Default value is ICRSW=0.

IDL1 Switches on writing of most variables to file IDL1 for later processing with IDL (Interactive Data Language). See section 13. Default value is IDL1=1.

IDLNY Switches on writing of frequency dependent information to file IDLNY. This file will be very large for large model atoms with many transitions. Default value is IDLNY=0.

IDLCNT Switches on writing of contribution functions to file IDLCNT. Default value is IDLCNT=0.

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