TLUSTY — A User's Guide

Version 195

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1 INTRODUCTION

The present set of computer programs is a package designed to accomplish a wide range of stellar spectroscopic diagnostics. In its maximum configuration, the user may start from scratch and calculate a model atmosphere of a chosen degree of complexity, and end with a synthetic spectrum in a wavelength region of interest for an arbitrary stellar rotation and an arbitrary instrumental profile.

The basic component of the package is TLUSTY, the program for calculating plane-parallel, horizontally homogeneous model stellar atmospheres in radiative and hydrostatic equilibrium. Departures from local thermodynamic equilibrium (LTE) are allowed for a set of occupation numbers of selected atomic and ionic energy levels. The program also allows for convection. The most important feature of the new version of the program is that it allows for a fully consistent, non-LTE metal line blanketing.

The second basic program is SYNSPEC, which is a program for calculating the spectrum emergent from a given model atmosphere. It has been written particularly to synthesize spectra from atmospheres calculated using TLUSTY, but may also be used with other model atmospheres as input (e.g. Kurucz' ATLAS models). The program is complemented by program ROTINS which calculates the rotational and instrumental convolutions for the net spectrum produced by SYN-SPEC.

Finally, there is a number of interface and utility programs. They provide graphical interface for plotting output models, the convergence log etc. (written in IDL and/or Mongo). Similarly, there is graphical interface SYNPLOT (written again in IDL), which enables the user an interactive work with SYNSPEC and its utility programs (computing the spectrum, plotting it, performing various convolutions, and identifying and annotating predicted lines).

The following document is a brief guide to the operation of the program, to preparing the required input and to understanding the resulting output, and to illustrate some of the options. However it is by no means exhaustive. We describe both basic programs, TLUSTY and SYNSPEC, in separate manuals. The present one describes the basic program TLUSTY; SYNSPEC is described in detail by Hubeny, Lanz, Jeffery (1994).

We stress that the set of programs does not represent a rigid structure of standard programs; instead, it is a highly dynamic set in a permanent state of gradual development. The version being described here is TLUSTY195. The previously distributed User's Guide described TLUSTY version 185.

The most significant difference between the previous and the present version is, besided an upgrade of several numerical algorithms, the change of the format of input data. The handling of large volumes of atomic data is now much easier. The program retained the option of accepting the "old" input data; however, a new user to encouraged to start with the "new" system of input,

which is much easier to set up. The basic feature of the new input data format is that there is only a very short standard input file, which specifies i) the very basic parameters for which no reasonable default values can be specified; ii) names of files where the atomic data for the individual ions are stored; and iii) the name of file where optional "non-standard" parameters are set up. Non-standard parameters are defined as such for which the program assigns default values, which are optimum for most applications, while may be changed if required for a particular special application.

Finally, we mention that an analogous set of programs also exists for accretion disks; a program for computing the vertical structure of a disk, TLUSDISK. This programs is not currently distributed through CCP7, but an interested reader may directly contact I. Hubeny to obtain a copy.

2   GENERAL CHARACTERISTICS

The basic features of the program are the following:

1. The program solves the basic equations (radiative transfer, hydrostatic equilibrium, radiative equilibrium, statistical equilibrium, charge and particle conservation) by the so-called hybrid CL/ALI method (Hubeny and Lanz 1995). This method combines advantages of its two basic constituents, a high convergence rate of the method of complete linearization, first introduced by Auer and Mihalas (1969), and a low computer time per iteration as the Accelerated Lambda Iteration (ALI) method, introduced by Cannon (1973) – for a review, see Hubeny (1992).

2. Not all of the basic equations have to be actually solved. The program has options for omitting some of the equations, keeping the corresponding quantities fixed. For instance, one may keep the temperature fixed and skip the radiative equilibrium equation (all the other equations being solved exactly); this corresponds to calculating the so-called semi-empirical models.

3. The program is fully data oriented as far as the choice of atomic species, ions, energy levels, transitions, and opacity sources is concerned. We stress that there are no default opacities built in (only some default formulae for various cross-sections are included – see below).

4. The final NLTE model is usually calculated by a standard procedure which consists of calculating consecutively a series of models with increasing complexity: first an LTE model starting from an LTE-grey model, than a NLTE model where all lines are assumed to be in detailed radiative balance (usually denoted as NLTE/C models; C stands for "continua-only"); and finally a model where also lines are considered explicitly. The last step may actually be composed of several partial steps, with gradually increasing number of lines considered. In some cases, certain steps may be skipped. For instance, for line blanketed models, it is sometimes easier to go from an LTE model directly to NLTE model with lines, etc. Except for the LTE-grey model, which is calculated from scratch, an initial estimate of the model is required. This is usually a converged model from the previous step, but it may also be a model taken from literature deemed to be a reasonable initial estimate.

5. The code is written in standard FORTRAN77, making it highly portable.

A detailed description of TLUSTY is given by Hubeny (1988). This paper describes the basic concepts, equations, and numerical methods used. However, because the program has developed considerably since 1988, the description presented in this paper is in many places obsolete. The

major new developments are described in detailed in Hubeny and Lanz (1992) – the Ng and Kantorovich accelerations; and, more importantly, in Hubeny and Lanz (1995) – the hybrid CL/ALI method, and the concept of superlevels and supertransitions treated by means of an Opacity Distribution Functions (ODF). Treatment of occupation probabilities, merged levels, and corresponding ODF is described by Hubeny, Hummer, Lanz (1994).

The new developments are virtually always downward compatible; i.e. all the options which were allowed in the older versions are preserved in a newer version. In other words, the newer versions only add new features, but do not delete the existing ones. Below, we list the most important modifications.

- Incorporation of the hybrid CL/ALI scheme (Hubeny and Lanz 1995).

- Incorporation of preconditioning of statistical equilibrium after Rybicki and Hummer (1992).

- Possibility of using the Discontinuous Finite Element (DFE) scheme for a formal solution of the transfer equation (Castor, Dykema, Klein 1992).

- Improved treatment of the radiative equilibrium equation, described by Hubeny and Lanz (1995).

- Incorporation of the occupation probability formalism (Hummer and Mihalas 1988), and its extension to NLTE situations; a detailed treatment of the line merging near the series limits (Hubeny, Hummer, and Lanz 1994).

- Acceleration algorithms (Kantorovich variant of the Newton-Raphson method; and the Ng acceleration), described in detail by Hubeny and Lanz (1992).

- Improved treatment of various physical features:

  - Convection (although still not working reliably)
  - External irradiation

- A number of various coding improvements and changes:

  - A loop over frequency points is now systematically coded as the outermost loop. This saves a large amount of memory, and allows a more efficient evaluation of opacity, emissivity, and their derivatives.
  - Full overlap of lines is allowed for.
  - Introduction of various options which enable the user not to linearize all populations (fixed or updated populations; fixed or updated b-factors).

Although considerable effort has been devoted to eliminate errors in the code, there is by no means a guarantee that it is error free. The user is thus warned against using program as a "black box". It would be highly appreciated if any errors detected by the user, and any comments or suggestions for an improvement, are communicated to I. Hubeny (Internet address: hubeny@stars.gsfc.nasa.gov, or hubeny@tlusty.gsfc.nasa.gov).

Compiling and linking

The program is distributed as several files. The largest is `TLUSTYnnn` where `nnn` represents the current version number. In the following text, we take 195 for the current version number. Communication between subprograms is principally carried out through labeled common blocks. To allow for the program to be scaled (re-dimensioned) easily, arrays are dimensioned by parameter constants. The arrays and parameters are defined using INCLUDE files

```
IMPLIC.FOR
BASICS.FOR
ATOMIC.FOR
MODELQ.FOR
ITERAT.FOR
ARRAY1.FOR
ODFPAR.FOR
ALIPAR.FOR
```

The INCLUDE files have to reside in the same directory as the `TLUSTY185` file, and, under UNIX, their names *must* be in capital letters, e.g. `BASICS.FOR`.

The basic parameters defining array dimensions appear in INCLUDE file `BASICS.FOR`. The first `PARAMETER` statement there contains the most important parameters; they have the following meanings:

MATOM	maximum number of explicit atoms
MION	maximum number of explicit ions
MLEVEL	maximum number of explicit levels
MLVEXP	maximum number of explicitly linearized levels
MMCDW	maximum number of levels with pseudocontinuum
MMER	maximum number of "merged" levels
MTRANS	maximum number of all transitions which are somehow taken into account
MDEPTH	maximum number of depth points
MFREQ	maximum number of frequency points
MFREX	maximum number of linearized frequencies
MFREQL	maximum number of frequencies per line
MITJ	maximum number of overlapping lines
MLINFR	maximum number of lines at given frequency
MSMX	size of largest matrix kept in memory in SOLVE
MTOT	maximum number of model unknowns (ie. maximum dimension of vector PSI)

The program checks whether the current values are less than the corresponding maximum dimension, and stops if there is a conflict.

The convention is that the names beginning with `M` designate the maximum dimension; the analogous names beginning with `N` then denote the current values; for instance `MATOM` is the dimension of the arrays containing information about explicit atoms (stored in the INCLUDE file `ATOMIC.FOR`), while `NATOM` is the current, actual number of explicit atoms, etc. The only exception from this rule is `MDEPTH` and corresponding `ND` for the maximum and actual number of discretized depth points.

The compilation and linking is done as follows:

- Under VMS:

```
FOR[/G_FLOAT] TLUSTY195
LINK TLUSTY195
```

The option /G_FLOAT, which increases the exponent range, is an recommended option on VAXes to be used for compiling because it is in some cases crucial for a successful convergence of the modeling procedure.

- Under UNIX:

```
f77 [-O4] [-static] [-Nl100] tlusty195.f
```

where the option "-Nl100" is sometimes needed under a SUN operation system (increases the number of continuation lines to 100); the option "-static", which was needed to be under Ultrix (older DEC workstations), indicating a static allocation of memory. It is a now default at most implementations. Similarly, the optimization (the option "-O4") is a default at most workstations. If not, the optimization should be switched on since it improves the performance of the code considerably.

- Under Unicos (Cray YMP):

Compiling and linking may be done together by

```
cf77 -Wf"-a static" tlusty195.f
```

Again, the INCLUDE file names must appear in capital letters. Another change which is recommendable is to modify the INCLUDE file IMPLIC.FOR from

```
IMPLICIT REAL*8 (A-H),(O-Z), LOGICAL*1 (L)
```

used under VMS and UNIX, to

```
IMPLICIT REAL (A-H),(O-Z), LOGICAL (L)
```

because Cray has a longer wordlength, and the use of REAL*8 slows down the execution significantly. Also, it is recommended to replace the ordinary matrix inversion routine MATINV by a Cray-specific, highly vectorized routine MINV from the standard library LINPACK (or analogous), as indicated in the program.

Reducing the size of the executable file

is accomplished by reducing some of the above parameters specifying array dimensions (in "include" file BASICS.FOR). If the problem at hand does not allow one to reduce important physical parameters, like MFREQ, MDEPTH, MLEVEL, MTRANS, etc., because the user needs the specified values, one may still reduce MSMX to 1 (matrices of complete linearization are not kept in memory but stored at temporary scratch files). This does save some memory (original MSMX × MSMX × ND × 3 words), with a relatively insignificant increase of computer time (of the order of 10 − 20%).

3 GENERAL SCHEME OF THE INPUT

As mentioned above, version 195 of TLUSTY allows for two different formats of input data:

- **"Old" format** – the format of input data is the same as in previous versions, i.e. there are two basic input files, plus one additional input file – the Unit 1 input:

  - Unit 1 — The basic control file, containing just one single number, specifying whether the subsequent input is in the "old" or "new" format. To switch on the old input format, this file should contain one single non-zero number.
  - Unit 5 — Main control data – one big file with all parameters.
  - Unit 8 — A starting model atmosphere (if needed).

- **"New" format** – The basic feature of the new input data format is that there is only a very short standard input file, which specifies i) the very basic parameters for which no reasonable default values can be specified; ii) the names of files where the atomic data for the individual ions are stored; and iii) the name of the file where optional "non-standard" parameters are set up. Non-standard parameters are defined as those for which the program assigns default values, which are optimum for most applications, but should be changed as required for a particular special application.

  - Unit 1 — The basic control file, containing just one single number, specifying whether the subsequent input is in the "old" or "new" format. If this number is 0, or if the file is missing altogether, the programs assumes the "new" input format.
  - Unit 5 — Main control data – a short file with only the most important parameters, and filenames of other files;
  - Files containing atomic data for the individual ions.
  - File containing non-default values of the non-standard parameters
  - Unit 8 — A starting model atmosphere (if needed).

All the input files are ASCII files to enable easy portability. All the `READ` statements use a free format. Moreover, Unit 5 may contain comment lines; TLUSTY understands a line beginning by * or ! as comment. The structure of these files is explained in detail below.

In the following three sections we describe the "new" system of input in detail. In Sect. **??**, we give a brief description of the "old" format, which is maintained in the program only for downward compatibility. The description of the old input format is by no means exhaustive; the user who is familiar with the old format, and would wish to consider some involved options of the program, may still do that by modifying the "old" input data, but is encouraged to make a gradual transition to the "new" format of input.

4 STANDARD INPUT IN THE "NEW" FORMAT

We now turn to a detailed description of the individual input parameters. The standard input is composed of four basic blocks:

4.1 First block – Basic Parameters

This block contains only three lines of input.

1st line:

TEFF – effective temperature [K]

GRAV – $\log g$ [cm s^{-2}]

2nd line:

LTE – a logical variable indicating whether an LTE model is going to be calculated.
    = .TRUE. – LTE model is calculated
    = .FALSE. – NLTE model is calculated

LTGRAY – a logical variable indicating whether an LTE-grey model is calculated at the beginning as a starting approximation for the linearization iterations.
    = .TRUE. – LTE-gray model is calculated as a starting model;
    = .FALSE. – LTE-gray model is not calculated; the user has to supply a starting model atmosphere – the Unit 8 input.

3rd line:

FINSTD – a character variable (up to 20 characters) with the name of file containing the values of non-standard parameters.
    = '' (null string) – all non-standard variables are taken with their default values – see the next section.

4.2 Second block – Frequencies

This block may contain just one line, in which case the frequency points and quadrature weights are set up automatically by the program following the general specifications given by the non-standard parameters. Otherwise, this block may contain the explicit values of all the frequency points and weights (set up by the user), exactly as in the previous versions. We stress that the frequency points set up here are generally those describing the continua; the frequency points in lines (if these are considered) are set up by default by the program.

Automatic setup of frequencies

In this case, there is only one input line in this block, containing just one number:

NFREAD – an indicator of the number of frequency points:
    > 0 – the program sets up the continuum frequencies automatically. In this case, the program always sets two frequencies near discontinuities corresponding to the bound-free transitions form all explicit levels, plus approximately NFREAD frequencies in between, plus about 20 points in the high- and low-frequency tails of the spectrum. The endpoints of the high- and low-frequency tails are defined by a non-standard parameter FRCMAX; the minimum by the non-standard parameters FRCMAX and FRCMIN (i.e. they may be changed by a corresponding specification in the input file FINSTD).
    < 0 – the program reads frequency points and weights from the standard input. In this case, abs(NFREAD) is the number of frequency points to be read.

In the automatic setup of frequency points, all the frequency points are treated by default in the ALI mode (i.e. IJALI=1 for all these frequency points). To change it, one employs parameters IFR0 and IFR1 for the appropriate bound-free transitions – see § **??**.

Explicit input of frequencies

In this case, there are abs(NFREAD) additional input records in this block. Each record contains the following parameters

FREQ – frequency (in Hz)

W – corresponding frequency quadrature weight

WCH – the "partial" quadrature weight:
$= 0$ – if the point is an interior point of a Simpson integration interval;
> 0 – for a boundary point of any integration domain (i.e. all points except interior points of a Simpson integration). In this case the weight W(IJ) is given by a sum of two contributions; the one from the higher frequency side, and the one from the lower frequency side. WCH had then the meaning of the lower frequency side contribution.
This quantity is used only in the non-overlapping mode (i.e. IOVER = 0), where the integration weight at the edge point of a continuum transition (program allows one or more transitions to have the same edge point), which appears in evaluating of radiative rates, is given by W(IJ)-WCH(IJ). In this mode, WCH is also used for setting the so-called subtraction weights (see CORRQW and CORRWM; detailed description is in Hubeny & Lanz 1995).

IJALI – basic switch of the hybrid CL/ALI method:
$= 0$ – the frequency point is explicitly linearized;
> 0 – the frequency point is treated by the ALI scheme (the so-called ALI point).

Notes:
i) There is a separate program SETFRE which generates the above described input for the continuum frequency points. This program is a part of the package. However, since version 195 is able to produce the frequency points automatically, program SETFRE is somewhat obsolete.

ii) Although the frequency points read in this block are referred to as "continuum" frequency points, they may also describe some selected lines. If a line has a full set of points already specified within the NFREAD frequencies, the corresponding input for this line should be set in such a way that the frequency points for this line will not be set up again. However, we stress again that in the overwhelming majority of uses of the program, the frequency points discussed above should be selected to cover only the continua; the frequency points in lines are usually set up by the program (see below). This is usually a highly recommended option.

iii) If the frequency points are set up manually, it must be kept in mind that the frequency points in continua *must* be ordered by decreasing frequencies. The frequency points in individual spectral lines (usually set up by the program) may then be ordered quite arbitrarily.

iv) We stress that there is no universal recipe to chose which frequency points are linearized. An optimum choice can be found with an extensive experimentation, which is almost never worth it. The most reasonable strategy is simply to set a few (2-4) frequency points in a few (1 - 3) most opaque continua (this points immediately shortward of the edges) to be linearized. In some cases, it is not necessary to select any point to be linearized.

4.3   Third block – Explicit atoms

This block is analogous to the input block for atoms used in the previous versions, but it is significantly simplified. The block contains one record with a value of NATOMS, and then NATOMS

analogous records for the individual species; each containing three parameters: MODE, ABN, MODPF. The order of individual records *must* exactly follow the atomic number (i.e. H, He, Li, Be, B, C, N, O, etc.).

Generally, a chemical element, hydrogen through zinc, can be considered in one of the three following options:

1. explicitly – some of energy levels of some of its ionization states are considered explicitly, ie. their populations are determined by solving statistical equilibrium.

2. implicitly – the atom is assumed not to contribute to opacity; but is allowed to contribute to the total number of particles and to the total charge; the latter is evaluated assuming LTE ionization balance, ie. by solving a set of Saha equations.

3. not considered at all.

The description of the individual input parameters follows:

NATOMS – the highest atomic number of an element that is considered (explicitly or non-explicitly).
< 0 – then abs(NATOMS) has the meaning as above, but all the partition functions of all species considered by the Opacity Project are evaluated from the Opacity Project ionization fraction tables, regardless of the parameter MODPF (see below).

MODE – a specification of the mode of treatment of the given species:
$= 0$ – if the element is not considered (option 3);
$= 1$ – if the element is non-explicit (option 2);
$= 2$ – if the element is explicit (option 1).

ABN – a specification of abundance of the given species:
$= 0$ – the solar abundance is assumed;
< 0 – a non-solar abundance is assumed, abs(ABN) has now the meaning of the abundance expressed as a multiple of the solar abundance (i.e. -0.1 means $1/10$ of solar, -5 means 5 times solar abundance, etc.);
> 0 – a non-solar abundance ABN is assumed, expressed as $N(\text{elem})/N(\text{H})$, i.e. relative to hydrogen by number;
$> 10^6$ – non-homogeneous (depth-dependent) abundance is assumed. In this case, the following lines should contain the individual values of the abundance (relative to hydrogen by number), for all depth points ID=1,ND.

MODPF – a flag indicating a mode of evaluation of the partition functions for the given species. Notice that this may be overwritten by coding NATOMS as negative – see above.
$= 0$ – a standard evaluation of the partition functions, after Traving, Baschek, and Holweger (1966) – subroutine PARTF
> 0 – the partition functions evaluated from the Opacity Project ionization fraction tables.

Notice that unlike the previous versions, this input does not contain any indices of the first and the last level of the explicit species. They are set up by the program.

4.4 Fourth block – Explicit ions

The input block for the ionic parameters, both the atomic and the computational ones, is greatly simplified in the "new" format of input. For each ion, including the highest ionization degree of a given species, there is one input record containing the following parameters:

IATII - the atomic number of the parent species of the ion (i.e. 1 for hydrogen, 2 for all ions of helium, etc.).

IZII – the charge of the ion (0 for neutrals, 1 for once ionized, etc.).

NLEVS – a number of energy levels considered explicitly.

ILAST – an indicator whether the given ion is the highest considered ionization degree:
$= 0$ – the ion is not the highest ion of the parent species; the subsequent input record will contain parameters for the next higher ion;
> 0 – the ion is the highest ionization degree of the parent species.
$= 1$ – the program assigns the correct statistical weight of the ground state of this ion automatically;
$\neq 1$ – has the meaning of the statistical weight of the ground state of this ion;
< 0 – indicates the last record of the block of the Explicit ions input.

ILVLIN – an indicator of changing the treatment of a whole group of bound-bound transitions, regardless of the detailed input for transitions. ILVLIN has the meaning that all lines with the relative index of the lower level which is smaller than ILVLIN are considered in detailed radiative balance. The relative index counts the levels within the ion; i.e. the ground state of the ion has relative index 1, the last considered level the index NLEVS. For instance, setting ILVLIN=2 will put all lines originating from the ground state to the detailed radiative balance, which is often a useful option. Setting ILVLIN > NLEVS will put all lines of the ion to detailed balance.
This option enables one to consider the same ionic input files for LTE, NLTE/C, and NLTE/L models.

NONSTD – an indicator of an additional input record, to change specific "non-standard" parameters for the ion (those having assigned default values that provide optimum for most of applications), or to provide necessary filenames for treating ions for which the Opacity Distribution Functions (ODF) are considered (typically the iron-peak elements).
$= 0$ – no change of non-standard parameters is required;
> 0 – additional record with "non-standard" parameters – see below;
< 0 – additional record with ODF units and filenames – see below.

TYPION – a character*4 variable containing a descriptive label, e.g. 'He 2' for He^+, etc.

FILEI – a character variable containing the filename where the detailed input of parameters for explicit level, bound-free transitions, and bound-bound transitions are stored. The structure of this file is described in detail in Sect. 6.

Note: The number of levels considered for the ion, NLEVS, *must not* exceed the number of levels given in the file FILEI. However, NLEVS may be smaller; in such a case the current run will select NLEVS lowest levels from the file FILEI.

4.5 Optional, non-standard parameters for the individual ions

If the parameter NONSTD of the standard input (see the previous section) is coded as positive, the programs reads the additional record with the four following parameters:

IUPSUM – mode of evaluation of total population of higher, non-explicit, LTE energy levels of the ion – the so-called upper sum:
$= 0$ – calculated by means of the partition function (see Hubeny 1988);
> 0 – calculated as a sum of populations of hydrogenic levels starting with the quantum number next to the highest explicit level and ending with IUPSUM;
< 0 – the occupation probability form (Hubeny, Hummer, & Lanz 1994).
DEFAULT: IUPSUM$=-100$ for hydrogen; IUPSUM$=0$ for other species.

ICUP – mode of considering a "modified collisional ionization rate", ie. that allowing for collisional excitation into, and collisional deexcitation from, higher, non-explicit, LTE energy levels of the ion:
$= 0$ – this contribution is neglected;
> 0 – calculated as a sum of contributions of rates into and from averaged (hydrogenic) levels starting with the quantum number next to the highest explicit level and ending with ICUP.
DEFAULT: ICUP$=16$ for all ions but He II; ICUP$=32$ for He II.

MODEFF – mode of evaluating the free-free cross-section:
$= 0$ – free-free opacity is neglected;
$= 1$ – hydrogenic cross-section with the Gaunt factor set to unity;
$= 2$ – hydrogenic cross-section with the exact Gaunt factor;
< 0 – non-standard expression, given by the user supplied subroutine `FFCROS`.
DEFAULT: MODEFF$=2$ for H I and He II; MODEFF$=1$ for all other ions.

NFF – mode of considering "modified free-free" opacity, ie. allowing for the photoionization from higher, non-explicit, LTE energy levels of the ion:
$= 0$ – this contribution is neglected;
> 0 – principal quantum number of the first non-explicit level.
DEFAULT: NFF$=0$

If the parameter NONSTD of the standard input (see the previous section) is coded as negative, the programs reads the additional record with the four following parameters:

INODF1, INODF2 – unit numbers for the ODF input. If they are zero, the program assigns the unit numbers automatically.

FIODF1, FIODF2 – filenames of the ODF input (the files, which in the old input format, with e.g. INODF1=31 and INODFF=32 were called `fort.31` and `fort.32`)

FIBFCS – the name of the file containing the photoionization cross-sections for the individual superlevels (the file, which in the old input format, e.g. for IFANCY=62 – see below – was called `fort.62`). The parameters IFANCY has again to be set to a value between 50 and 99 to switch on reading cross-sections from a previously created file, but unlike the old format of input, IFANCY does not now have the meaning of a unit number.

Detailed description of the ODF input files is given in Sect. xxx.

4.6 An example

A simple LTE model atmosphere with $T_{\mathrm{eff}} = 35{,}000$ K, $\log g = 4$, composed of H and He only, may be constructed by TLUSTY195 by coding the standard input as follows:

```
35000. 4.0          ! TEFF, GRAV
T  T                ! LTE,  LTGRAY
','                 ! no change of general non-standard parameters
*----------------------------------------------------------------
* frequencies
50                  ! NFREAD
*----------------------------------------------------------------
* data for atoms
*
 2                  ! NATOMS
* mode abn modpf
    2   0   0
    2   0   0
*----------------------------------------------------------------
* data for ions
*
*iat    iz   nlevs  ilast ilvlin  nonstd typion  filei
*
    1    0    9       0    100       0    ' H 1' 'h1.dat'
    1    1    1       1     0        0    ' H 2' ' '
    2    0    14      0    100       0    'He 1' 'he1.dat'
    2    1    14      0    100       0    'He 2' 'he2.dat'
    2    2    1       1     0        0    'He 3' ' '
    0    0    0      -1     0        0    '     ','
*
* end
```

where the atomic data for H, He I, and He II are stored in files `h1.dat, he1.dat, he2.dat,` respectively. Here we assume that the models atoms contain 9, 14, and 14 levels of these ions, respectively. H II and He III are taken as 1-level ions. Notice that there are no additional input files associated with the highest ions, H II and He III.

The corresponding NLTE/C (continua only) model may be constructed with virtually the same standard input; the only change is replacing the second record by

```
F  F                ! LTE,  LTGRAY
```

and the final NLTE/L (NLTE with lines), considering all lines of H and He explicitly, by modifying the fourth block as follows

```
*
*iat    iz   nlevs  ilast ilvlin  nonstd typion  filei
*
    1    0    9       0     0        0    ' H 1' 'h1.dat'
    1    1    1       1     0        0    ' H 2' ' '
    2    0    14      0     0        0    'He 1' 'he1.dat'
```

```
2     1     14       0        0        0     'He 2' 'he2.dat'
2     2     1        1        0        0     'He 3' ' '
0     0     0       -1        0        0     '     ' ' ' '
```

The frequency points in all cases are set up automatically, with the default values of the highest frequency, (such as $h\nu_{\max}/kT_{\mathrm{eff}} = 30$ – see the next Section), the lowest frequency $\nu_{\min} = 10^{12}$. The number of frequency points is approximately $50+2\times(9+14+14)+20 = 144$ (i.e. NFREAD + twice the number of levels from which a bound-free transition can occur + about 20 points at the short- and long-wavelength tails); the actual number of points set up by the program is 143.

5   GENERAL NON-STANDARD PARAMETERS

There are about 90 different non-standard parameters. We repeat that a non-standard parameter is defined as such for which the program assigns a default value, which provides the optimum value for most applications, or the most reasonable value. A small part of non-standard parameters are actual physical parameters, like the convective mixing length, or the microturbulent velocity, which are zero for most applications. However, the majority of non-standard parameters are various computational flags and switches which specify the detailed setup of the numerical method. Notice that the overall degree of sophistication of the resulting model atmosphere is determined by the ionic input files, described in the subsequent section. The non-standard parameters discussed in this section, with the exception of the physical parameters mentioned above, will mostly influence the numerical performance – the rate of convergence (or a lack thereof!), the total computer time, a numerical accuracy, a degree of auxiliary output, etc.

We divide all the non-standard parameters into the following 12 categories.

1. Auxiliary physical parameters

2. Automatic setup of frequency points

3. Flags for specifying the starting model atmosphere

4. Specification of the LTE-gray model

5. Flags for the numerical setup of the radiative transfer equation and the approximate Λ operator

6. Flags for selecting a treatment of the statistical equilibrium equation

7. Parameters for the global iteration loop control

8. Parameters for setting up the linearization matrices

9. Parameters defining the additional opacities

10. Parameters defining the numerical treatment of convection

11. Parameters specifying the global acceleration schemes

12. Miscellaneous auxiliary parameters

The file, whose name is specified by the standard parameter FINSTD (see the previous Section), contains a list of the non-standard parameters to be changed from their non-standard values. The input format is very simple, namely

```
     PARAM1=VALUE1,PARAM2=VALUE2,...
```

where `PARAM1`, etc., are the names of the parameters as specified below, and `VALUE1`, etc, are the corresponding numerical values of the parameters. The individual entries are delimited by one of the following special characters: coma (`,`), space, left or right bracket (`(` or `)`), asterisk (`*`), slash (`/`), or carriage return. The parameters may appear in any order. If a parameter does not appear in the list, its default value is adopted by the program. The name of a parameter should be coded with capital letters. The numerical values `VALUE1`, etc., may be up to 6 character long. This system of input was adopted from Carlsson's program MULTI (Carlsson 1976); we have used and modified his routines GETWRD and RINPUT.

Aa an example, to select the Discontinuous Finite Element scheme for representing the radiative transfer equation, setting the number of the internal iterations of the formal solution (the so-called lambda iterations) to 3, and requiring the Kantorovich acceleration starting from 8th iteration, we have to set up the non-standard input file as follows

```
ISPLIN=5,NLAMBD=3,ITEK=8
```

Notice that by coding, for instance `ISPL=5`, or `isplin=5`, one would not effectuate the change of the value of parameter `ISPLIN` to 5; instead it would keep its default value, `ISPLIN=0`.

In the rest of this Section, we will describe all the individual non-standard parameters in detail, including their default values.

5.1 Auxiliary physical parameters

HMIX0 – the mixing length parameter:
> 0 – convection is considered; HMIX0 has the meaning of mixing length;
= 0 – convection is suppressed, but the adiabatic and radiative gradients are calculated and printed;
< 0 – convection is suppressed and no gradients are calculated.
DEFAULT: HMIX0=-1.

VTB – microturbulent velocity; in km s^{-1} or cm s^{-1} (a numerical value $< 10^3$ indicates that the microturbulent velocity is expressed in km s^{-1}).
DEFAULT: VTURB=0.

TRAD – the external irradiation parameter:
= 0 – no external irradiation is considered;
> 0 – the external irradiation is considered; the irradiation intensity is assumed to be given by $I_\nu^{\mathrm{irrad}} = W\,B_\nu(T^*)$, where W is the dilution factor, B the Planck function, and T^* the characteristic temperature of incoming radiation. The parameter TRAD has then the meaning of T^*.
< 0 – the irradiated intensity is read for all frequency points.
DEFAULT: TSTAR=0.

WDIL – the dilution factor W (has a meaning only if TSTAR > 0).
DEFAULT: WDIL=1.

5.2 Automatic setup of frequency points

FRCMAX – the maximum frequency.
= 0 – maximum frequency is set up such as $h\nu_{\max}/(kT_{\mathrm{eff}}) = 30$.
DEFAULT: FRCMAX=0.

FRCMIN – the minimum frequency.
= 0 – the minimum frequency is set to 10^{12} s^{-1}.
DEFAULT: FRCMIN=10^{12}

FRLMAX – the maximum frequency in the line transitions.
= 0 – the maximum frequency in the line transitions is set to FRCMAX.
DEFAULT: FRLMAX=FRCMAX

FRLMIN – the minimum frequency in the line transitions.
= 0 – the minimum frequency in the line transitions is set to 10^{13} s^{-1}.
DEFAULT: FRLMIN=10^{13}

NFTAIL – number of frequency points in the high-frequency "tail", i.e. the region between the highest frequency FRMAX and the photoionization discontinuity with the highest frequency. The integration is done by the Simpson formula, so that NFTAIL must be an odd number. Specifically, the intergation is done by two Simpson integrations, dividing the total tail region into two parts, each part is done by a (NFTAIL/2+1)-point Simpson integration, and the part nearer to the photoionization edge is DFTAIL times the total interval. This allows one to consider denser grid of frequency points just blueward of the highset-frequency disconti-nuity, which yields more accurate evaluation of the photoionization rate of the corresponding transition.
DEFAULT: NFTAIL=21

DFTAIL – see above.
DEFAULT: DFTAIL=0.25

5.3   Flags for specifying the starting model atmosphere

INTRPL – a switch indicating that the input model atmosphere has to be interpolated to a new depth scale to obtain the starting model. For a detailed discussion, see § **??**.
= 0 – no interpolation (i.e. the same depth grid in the input and current models);
> 0 – interpolation from the input depth grid to the current one; the actual interpolation scheme is the polynomial interpolation of the (INTRPL$-$1)th order;
< 0 – the starting model atmosphere is a Kurucz model.
DEFAULT: INTRPL=0

ICHANG – switch indicating a change of the explicit level structure between the input model atmosphere and the current run. It has an effect only for NLTE models. For a detailed discussion, see § **??**.
= 0 – no change of level structure (i.e. the same explicit levels, with the same overall indices, are considered in the input model and in the present model to be computed).
> 0 – change of the structure; a detailed additional input for each level of the present run is required;
< 0 – a "simple" change of the level structure – levels are only added, and only for new species.
DEFAULT: ICHANG=0

5.4   LTE-grey model input

TAUFIR – the Rosseland optical depth in the first depth point.
DEFAULT: TAUFIR=1.d-7

TAULAS – the Rosseland optical depth in the last depth point.
DEFAULT: TAULAS=3.16d2

ABROS0 – the initial estimate of the Rosseland opacity (per gram) at the first depth point.
DEFAULT: ABROS0=0.4

TSURF – a mode of evaluation of the surface temperature:
$= 0$ – surface temperature and the Hopf function are evaluated exactly;
> 0 – the value of surface temperature is set to TSURF, and the Hopf function is assumed to be constant, corresponding to TSURF.
DEFAULT: TSURF=0.

ALBAVE – frequency-integrated wind blanketing albedo;
DEFAULT: ALBAVE=0 (no wind blanketing)

DION0 – the initial estimate of the degree of ionization at the first depth point (=1 for completely ionized; =1/2 for completely neutral).
DEFAULT: DION0=1.

NDGREY – the number of depth points for evaluating LTE-grey model.
$= 0$ – NDGREY is taken to be ND-1
DEFAULT: NDGREY=0

IDGREY – a mode of determining the mass-depth scale to be used in the subsequent linearization:
$= 0$ – the depth grid DM (in $g\,cm^{-2}$) is evaluated as a column mass corresponding to Rosseland optical depths which are equidistantly spaced in logarithms between the first point TAUFIR and the last point TAULAS the last-but-one point is, however, set to TAULAS-1.
$= 2$ – the depth grid DM is evaluated as that corresponding to input values of Rosseland optical depth – array TAU0(ID), ID=1,ND
$= 1$ – similar, but now DM is evaluated as the mass corresponding to the Rosseland optical depths which are equidistantly spaced in logarithms between the first point TAU1 and the last-but-one point TAU2; the last point is TAUL (with TAU1, TAU2, and TAUL are additional input parameters). This option is similar to the option IDGREY=0, but now TAU1 and TAUL may be different from TAUFIR nad TAULAS.
DEFAULT: IDGREY=0

IPRING – a flag that controls diagnostic output of the LTE-gray model calculations:
$= 0$ – no output;
$= 1$ – only final LTE-gray model is printed;
$= 2$ – results of all internal iterations are printed;
DEFAULT: IPRING=0

NCONIT – a number of internal iterations for calculating the gray model with convection.
DEFAULT: NCONIT=10

IHM – if non-zero, negative hydrogen ion is considered in the particle and charge conservation in subroutine ELDENS;
DEFAULT: IHM=0

IH2 – if non-zero, hydrogen molecule is considered in the particle and charge conservation in subroutine ELDENS;
DEFAULT: IN2=0

IH2P – if non-zero, ionized hydrogen molecule is considered in the particle and charge conservation in subroutine ELDENS;
DEFAULT: IH2P=0

5.5 Flags for a numerical setup of the radiative transfer equation and evaluation the approximate Λ operator

ISPLIN – Mode of numerical representation of the radiative transfer equation.
= 0 – ordinary second-order Feautrier scheme
= 1 – spline collocation scheme
= 2 – Auer's fourth-order Hermitian scheme
= 3 – improved Feautrier scheme (Rybicki & Hummer 1991)
= 5 – Discontinuous Finite Element (DFE) scheme (Castor, Dykema, & Klein 1992)
DEFAULT: ISPLIN = 0

IRTE – mode of setup of the DFE method (effective only if ISPLIN=5). There are several options which have only historical significance, as they were used for testing.
DEFAULT: IRTE=3

IFALI – basic switch for treating the ALI mode:
= 0 – no ALI option, i.e. all frequency points are explicitly linearized; and all the "fixed-rates" transitions are treated as fixed (as in original TLUSTY – Hubeny 1988);
= 1 - 4 – ALI scheme, with some limitations. It has only a historical significance; it was used for testing purposes.
= 5 – full ALI scheme with diagonal Λ^*;
= 6 – full ALI scheme with tri-diagonal Λ^*;
DEFAULT: IFALI=5

JALI – switch determining the type of the Λ^* operator.
= 1 – Λ^* evaluated by the Rybicki-Hummer (1991) algorithm;
= 2 – Olson-Kunasz (1988) operator.
DEFAULT: JALI=1

IFRALI – a switch for a global change of the ALI mode of a whole group of frequency points
= 0 – the ALI mode for all frequencies is determined by the input for the individual frequency points and/or for individual transitions;
= 1 – all frequency points in lines are set to ALI mode (which overwrites an input for line transitions);
= 2 – all frequency points altogether are set to the ALI mode (i.e. the fully ALI scheme is forced regardless of other input).
DEFAULT: IFRALI=0

IBC – mode of the treatment of Λ^* at the lower boundary:
= 0 – Λ^* at depth points ND and ND-1 given by J_ν/S_ν
> 0 – Λ^* at depth points ND and ND-1 is computed exactly in the Rybicki-Hummer or Olson-Kunasz algorithms;
= 3 – in addition, all appropriate derivatives in the linearization are calculated exactly.
DEFAULT: IBC=3

ILMCOR – a mode of including the electron scattering contribution to the approximate lambda operator:

= 0 – the Lambda operator is defined as that acting on the source function $S = \eta/(\kappa + \sigma)$, i.e. $J = \Lambda[\eta/(\kappa + \sigma)]$; here η and κ are the thermal emission and absorption coefficients, and σ the scattering coefficient, $\sigma = n_e \sigma_e$, with σ_e being the electron scattering cross-section.
= 1 – the Lambda operator is defined as that acting on the thermal source function $S^{th} = \eta/\kappa$, i.e. $J = \Lambda[\eta/\kappa]$.
DEFAULT: ILMCOR=1

ILPSCT – a mode of including the electron scattering correction in the preconditioning scheme (subroutines RATSP1, ALIST1, etc.):
= 0 – the Lambda operator is defined as that acting on the thermal source function;
= 1 – the Lambda operator is defined as that acting on the source function of the form $S = \eta/(\kappa + \sigma)$.
DEFAULT: ILPSCT=0

ILASCT – a mode of including the electron scattering correction in the evaluation of the derivative of the source function with respect to the state parameters (T, n_e, and populations – subroutine ALIFR1):
= 0 – the Lambda operator is defined as that acting on the thermal source function;
= 1 – the Lambda operator is defined as that acting on the source function of the form $S = \eta/(\kappa + \sigma)$.
DEFAULT: ILASCT=0

DJMAX – the maximum relative change of the mean intensity in the internal ALI iteration loop for treating electron scattering in the case of DFE formal solution. Has an effect only if ISPLIN=5 and IRTE $\geq$ 3.
DEFAULT: DJMAX=0.001

NTRALI – the maximum number of iterations of the internal ALI iteration loop for treating electron scattering in the case of DFE formal solution. Has an effect only if ISPLIN=5 and IRTE $\geq$ 3.
DEFAULT: NTRALI=3

5.6 Flags for selecting a treatment of the statistical equilibrium equations

IFPREC – a flag for treating the preconditioning of the statistical equilibrium equations (after Rybicki & Hummer 1991):
= 0 – no preconditioning (i.e. a normal treatment of statistical equilibrium;
= 1 – a diagonal (local) preconditioning (after Rybicki & Hummer 1991) is switched on.
> 1 – tri-diagonal (non-local) preconditioning is switched on.
DEFAULT: IFPREC=1

IELCOR – the flag for turning off an iterative update of the electron density by solving iteratively a non-linear system of rate equations + charge conservation equation (subroutine ELCOR). IELCOR has the meaning of the serial number of the global iteration, starting from which the calls to ELCOR are switched off. Introduced for testing purposes only.
DEFAULT: IELCOR=100 (i.e. ELCOR is called always)

ICHC – switch for selecting the closing equation of the statistical equilibrium equation set:
= 0 – the closing equation is the particle conservation equation;
= 1 – the closing equation is the charge conservation equation.
DEFAULT: ICHC=0

IRSPLT – a switch for the mode of solution of the global system of rate equation set:
= 0 – statistical equilibrium equations for all species are solved simultaneously (with one big rate matrix);
= 1 – statistical equation is solved for one species at a time (i.e. the big rate matrix is split into partial rate matrices for the individual chemical species).
DEFAULT: IRSPLT=1

IATREF – a flag for setting up the reference atom.
Reference atom is the species to which all abundances are related (usually, but not necessarily, hydrogen).
= 0 – IATREF is set to 1 (i.e. the first explicit species).
DEFAULT: IATREF=1

MODREF – a flag for setting up the reference reference levels of the individual explicit atoms.
Reference level is the energy level for each species for which the statistical equilibrium equation is not written; instead, one considers the abundance definition equation. The indices of reference levels are stored in the array NREF(IAT), IAT=1,NATOM.
= 0 – NREF(IAT) is set to NKA(IAT), i.e. the highest ionization state of the species IAT.
= 1 – NREF(IAT) is determined by the program to be the index of ground level of the most populated ion of the species IAT.
= 2 – NREF(IAT) is set to index of the ground state of the second highest ionization state of the species IAT.
DEFAULT: MODREF=1

IACPP – switch for Ng acceleration of the preconditioned formal solution:
= 0 – no acceleration;
> 0 – acceleration is done first in the IACCP-th iteration of the formal solution, and is repeated every IACDP iterations;
Notice that if IACCP > NLAMBD (total number of iterations of the formal solution (called, inaccurately, lambda iterations), then no acceleration is performed.
DEFAULT: IACPP=7

IACDP – step for the Ng acceleration of the formal solution (see above).
DEFAULT: IACDP=4

IFLEV – a switch for globally changing the mode of treating the linearization of atomic level populations:
= 0 – the mode is specified by the input parameter IMODL (see the explanation of input block explicit levels), and is not changed;
> 0 – the mode is reset to all levels except the highest ionization stage to IMODL=1, i.e. the updated LTE. mode (see explanation in the input block of levels).
DEFAULT: IFLEV=0

IDLTE – a depth point below which all the explicit levels are forced to have LTE populations (even for NLTE models);
DEFAULT: IDLTE=1000 (no LTE populations are forced)

POPZER – a value of the ratio of a level population over the population of the most populated level of a given species, below which the population is declared to be "too small" and is set to 0. This option allows to consider many ionization degrees of an atom without running into

numerical problems connected with too small/large numbers.
DEFAULT: POPZER=1.e-20

IFPOPR – switch for treating a recalculation of populations.
= 0 – the original Auer-Mihalas scheme: after a completed linearization iteration, new populations (i.e. those obtained as $n^{\text{new}} = n^{\text{old}} + \Delta n$) are not used; instead one uses a new radiation field to compute new radiative rates, and the populations are determined by solving a rate equation. The option is kept for historical reasons; it is only useful for a pure complete linearization scheme.
> 0 – population directly coming from linearization are used. The individual values of IFPOPR switch on a different setup; again, these have only historical meaning; there is virtually no practical reason to change the default value.
DEFAULT: IFPOPR=4

5.7   Parameters for the global iteration loop control

IOVER – a flag for turning on the "line-overlapping" mode:
= 0 – no overlapping allowed for (only one line may contribute to opacity at any single frequency);
> 0 – a general line overlap is allowed.
DEFAULT: IOVER=1

ITLAS – a flag for turning off laser lines, i.e. those for which the absorption coefficient (= true absorption minus stimulated emission) becomes negative. Turning off laser lines means that the line absorption and emission coefficient are set to zero at depths where the absorption coefficient would be negative. ITLAS has the meaning of the global iteration number starting from which the laser lines are turned off (ITLAS=0 turns off laser lines from the very beginning).
DEFAULT: ITLAS=100

IFSUB – an outdated parameter. It is only useful in the non-overlapping mode, and is included for historical reasons anyway.
DEFAULT: IFSUB=0

NITER – maximum number of global linearization iterations.
DEFAULT: NITER=30

CHMAX – maximum relative change of the state vector. If all the relative changes of all state parameters at all depth points are below this value, the model is declared converged, and the execution stops after a finished formal solution.
DEFAULT: CHMAX= 10^{-3}

NLAMBD – number of "lambda" iterations of the formal solution.
DEFAULT: NLAMBD=2 for NLTE models; NLAMBD=1 for LTE models

ND – number of depth points

NELSC – a mode of treating the electron scattering by the Feautrier scheme (it has no meaning for the DFE scheme, ISPLIN ≥ 5):
= 0 – the electron scattering source function is treated exactly; i.e. the single-frequency

formal solution of the transfer equation contains an explicit angular coupling due to the J_ν-dependence of the electron scattering source function;

> 0 – the electron scattering source function is treated as the thermal source function, i.e. it is given through the current mean intensity J_ν. It is included for pedagogical and testing purposes only.

DEFAULT: NELSC=0

IHECOR – a mode of recalculating the hydrostatic equilibrium equation in the formal solution:

$= 0$ – no recalculation (i.e. the total particle density N is held fixed);

> 0 – the the total particle density N is recalculated.

DEFAULT: IHECOR=0

IBFINT – a mode of storing the photoionization cross-sections:

$= 0$ – means that cross-sections are stored for all frequency points;

$= 1$ – means that photoionization cross-sections are stored only for continuum frequencies, and are interpolated for line frequencies;

DEFAULT: IBFINT=1

IRDER – a mode of treatment of linearization of the statistical equilibrium equations in the ALI scheme:

$= 0$ – the rate equation in the ALI scheme are not linearized;

> 0 – the rate equation in the ALI scheme are linearized; there are several variants of neglecting specific derivatives, which are of historical significance as they were used for testing purposes;

$= 3$ – full linearization; all derivatives are calculated exactly.

DEFAULT: IRDER=3

ILDER – a flag for controlling evaluation of derivatives of recombination rates with respect to temperature. Introduced for testing purposes only.

$= 0$ – derivatives are calculated;

> 0 - derivatives are set to zero.

DEFAULT: ILDER=0

IBPOPE – a flag for controlling derivatives of the rate equations. Introduced for testing purposes only.

$= 0$ – derivatives of the rows of rate equations with respect to the mean intensity in the linearized frequency points are not calculated;

> 0 – derivatives are calculated.

DEFAULT: IBPOPE=1

CHMAXT – a parameter which enables to change the number of iterations of the formal solution (the so-called lambda iterations) when the model is almost converged. If the maximum of absolute values of relative changes of the temperature at all depths decreases below CHMAXT, the number of lambda iterations is set to NLAMT.

DEFAULT: CHMAXT=0

NLAMT – the reset number of lambda iterations – see above.

DEFAULT: NLAMT=1

5.8 Parameters for setting up the linearization matrices

The following parameters INHE, INRE, INPC, INSE, INMP, INDL each correspond to one equation and one model parameter – see below.

If INxx = 0, then the corresponding equation is not solved, and the corresponding quantity is thus held fixed.

If INxx > 0, the corresponding equation is solved, and the corresponding quantity is the (NFREQE+INxx)-th component of the vector PSI of unknown model parameters (the first NFREQE components are mean intensities of radiation in explicitly linearized frequency points).

INHE – a position of N; an index of the hydrostatic equilibrium equation.
    DEFAULT: INHE=1

INRE – a position of T; an index of the radiative equilibrium equation.
    DEFAULT: INRE=2

INPC – a position of n_e; an index of the number conservation equation (or the charge conservation equation, depending on parameter ICHC). In any case, it is the equation which determines the electron density.
    DEFAULT: INPC=3 (or INPC=4 for convective models)

INSE – a position of n_1, i.e. the first population; index of the first statistical equilibrium equation.
    DEFAULT: INSE=4 (or INSE=5 for convective models)

INMP – a position of n_m – massive particle number density; after Auer & Mihalas. The option is included for historical reasons only.
    DEFAULT: INMP=0

INDL – a position of Δ – the logarithmic gradient of temperature. It is used only for convective models.
    DEFAULT: INDL=0; or INDL=3 for convective models

NDRE – a parameter that defines a treatment of the radiative equilibrium equation (REE), namely a form of the superposition of the integral and the differential equation representations:
= 0 – a linear combination of both forms is used, after Hubeny & Lanz (1995). In this case, the form of the linear combination is given by parameters TAUDIV and IDLST, in such a way that:

- the integral form is used for depth points ID, ID=1,ND−IDLST;
- the differential form for depth points where the Roseland optical depth is smaller than TAUDIV.

> 0 – the coefficients are step functions with discontinuity at ID = NDRE, i.e.:
for depth points (ID=1,NDRE−1) – REE is treated as a pure integral equation;
for depth points (ID=NDRE,ND) – REE is treated as a pure differential equation.
DEFAULT: NDRE=0

TAUDIV – see above (effective only if NDRE=0)
    DEFAULT: TAUDIV=0.5

IDLST – see above (effective only if NDRE=0)
    DEFAULT: IDLST=5

5.9 Additional opacities

IOPADD – a switch for calculating additional opacities:
   = 0 – no additional opacities are calculated;
   > 0 – certain additional opacities are calculated, the user either employs existing expressions in OPADD, or add his/her own expressions into OPADD. In the former case, there are the following existing possibilities; the relevant opacity is evaluated if the values of the following switches are non-zero.
   DEFAULT: IOPADD=0

IRSCT – a switch for considering the Rayleigh scattering
   DEFAULT: IRSCT=0

IOPHMI – a switch for considering the H- opacity (both bound-free and free-free), assuming LTE. Note that H- can be considered as one of explicit ions, then the opacity is automatically calculated (in NLTE if such model is calculated). In this case one must code IOPHMI=0 in order not to calculate H- opacity twice.
   DEFAULT: IOPHMI=0

IOPH2P – a switch for considering the opacity of H_2^+ (molecular hydrogen ion)
   DEFAULT: IOPH2P=0

IOPHE1 – a switch for considering the approximate, hydrogenic, opacity of neutral helium given as a sum of bound-free transitions from averaged levels with principal quantum numbers between that next to the highest level considered explicitly and IOPHE1. Outdated, and included for historical reasons only.
   DEFAULT: IOPHE1=0

IOPHE2 – a switch for considering the approximate, hydrogenic, opacity of ionized helium given as a sum of bound-free transitions from averaged levels with principal quantum numbers between that next to the highest level considered explicitly and IOPHE2. Outdated, and included for historical reasons only.
   DEFAULT: IOPHE2=0

5.10 Parameters defining a numerical treatment of convection

ICONV – a flag to switch on the convection:
   = 0 – convection is neglected altogether;
   > 0 – convection is considered, and is linearized;
   < 0 – convection is taken into account, but is not linearized.
   DEFAULT: ICONV=0

IPRESS – a flag for treating the total pressure in the convection zone:
   = 0 – total pressure is held fixed when evaluating derivatives of the convective flux;
   = 1 – derivatives w.r.t. total pressure are calculated.
   DEFAULT: IPRESS=0

ITEMP – a flag for treating the temperature correction when the convection is taken into account:
   = 0 – a "new" temperature, obtained after a completed iteration of the complete linearization, is calculated as $T^{\rm new} = T^{\rm old} + \Delta(T)$ (as it is done without convection);
   = 1 – new temperature is calculated through DELTA in the convection zone;

= 2 – new temperature is calculated through DELTA everywhere.
DEFAULT: ITEMP=0

IPRINT – a flag that controls a diagnostic output for models with convection:
= 0 – no additional print, only final model is printed;
= 1 – the convective flux and the results of routine CONCOR are printed after each iteration.
DEFAULT: IPRINT=0

5.11 Acceleration parameters

IACC – a switch for the Ng acceleration procedure:
≤ 4 – Ng acceleration in the 7th, 10th, etc, iteration;
≥ 5 – Ng acceleration in the iterations ITER=IACC, IACC+IACD, IACC+2×IACD, etc.
≤ 0 – no Ng acceleration.
DEFAULT: IACC=7

IACD – a step for Ng acceleration – see above.
DEFAULT: IACD=4

ITEK – the iteration after which the Kantorovich method is set up
DEFAULT: ITEK=5

ORELAX – an over-relaxation coefficient.
DEFAULT: ORELAX=1.

5.12 Miscellaneous parameters

IWINBL – a switch indicating whether the wind-blanketing albedo is considered. Kept for historical reasons.
= 0 – wind blanketing is not considered > 0 – wind blanketing is considered, basically as in Abbott and Hummer (1985), slightly modified after Voels et al. (1988) to treat properly the angle-averaged albedos.
DEFAULT: IWINBL=0 (no wind blanketing)

NPGPOP – a switch that determines an amount of the level population diagnostic output:
= 0 – standard option – level populations are printed for 6 levels per page, consecutively by increasing index;
< 0 and > -10 – the same print of populations as for NPGPOP=0; but also unit 77 is created, equivalent to unit 7, in which a new model is appended after each completed linearization iteration;
< -10 - - the same print of populations as for NPGPOP=0; but also unit 77 is created, equivalent to unit 7, in which a new model is appended after each lambda iteration in each linearization iteration;
> 0 – non-standard option, in this case the array IIPR is read, which specifies which population are printed. An outdated option.
DEFAULT: NPGPOP=0

ICRSW – a flag indicating whether the collisional-radiative switching scheme (Hummer & Voels 1988) is considered:
= 0 – collisional-radiative switching not considered;

> 0 – collisional-radiative switching is considered; and
= 1 – with depth-independent switching parameter;
> 1 – with depth-dependent switching parameter.
DEFAULT: ICRSW=0

SWPFAC – the initial c.-r. switching parameter is given by
SWPFAC $\times$ min(collisional rate/radiative rate)
DEFAULT: SWPFAC=0.1

SWPLIM – has the meaning that if c.-r. switching parameter is larger than SWPLIM, then the program assigns c.-r. switching parameter = 1.
DEFAULT: SWPLIM=0.001

SWPINC – the increment of the switching parameters, defined by
switching parameter(actual) = switching parameter(previous) $\times$ SWPINC.
DEFAULT: SWPINC=3.

5.13   List of all non-standard parameters in alphabetic order

Here we give the list of all non-standard parameters in alphabetic order, including their default values.

ABROS0	0.4
ALBAVE	0
CHMAX	10^{-3}
CHMAXT	0
DFTAIL	0.25
DION0	1.
DJMAX	0.001
FRCMAX	0.
FRCMIN	10^{12}
FRLMAX	0.
FRLMIN	10^{13}
HMIX0	$-1.$
IACC	7
IACD	4
IACDP	4
IACPP	7
IATREF	1
IBC	3
IBFINT	1
IBPOPE	1
ICHANG	0
ICHC	0
ICONV	0
ICRSW	0
IDGREY	0
IDLST	5
IDLTE	1000

IELCOR	100
IFALI	5
IFLEV	0
IFPOPR	4
IFPREC	1
IFRALI	0
IFSUB	0
IH2	0
IH2P	0
IHECOR	0
IHM	0
ILASCT	0
ILDER	0
ILMCOR	1
ILPSCT	0
INDL	0 (or INDL = 3 for convective models)
INHE	1
INMP	0
INPC	3 (or INPC = 4 for convective models)
INRE	2
INSE	4 (or INSE = 5 for convective models)
INTRPL	0
IOPADD	0
IOPH2P	0
IOPHE1	0
IOPHE2	0
IOPHMI	0
IOVER	1
IPRESS	0
IPRING	0
IPRINT	0
IRDER	3
IRSCT	0
IRSPLT	1
IRTE	3
ISPLIN	0
ITEK	5
ITEMP	0
ITLAS	100
IWINBL	0
JALI	1
MODREF	1
NCONIT	10
ND	70
NDGREY	0
NDRE	0
NELSC	0
NFTAIL	21

NITER	30
NLAMBD	2 for NLTE models; NLAMBD = 1 for LTE models
NLAMT	1
NPGPOP	0
NTRALI	3
ORELAX	1.
POPZER	10^{-20}
SWPFAC	0.1
SWPINC	3.
SWPLIM	0.001
TAUDIV	0.5
TAUFIR	10^{-7}
TAULAS	316.
TRAD	0.
TSURF	0.
VTB	0.
WDIL	1.

6   INPUT FILES FOR THE INDIVIDUAL IONS

The input file contains information about three basic types of atomic data, namely:

1. Energy levels (i.e. level energies, statistical weights, etc.).

2. Bound-free transitions (modes of evaluation of the photoionization cross-section, collisional ionization rates, etc.).

3. Bound-bound transitions (necessary data for lines).

The structure of the input data in these files are quite analogous to the format used in the previous versions of TLUSTY. The essential difference is that in the previous versions the data were organized in such a way that all energy level data for all ions were packed together to form the energy level block, then the bound-free transitions data for all ions were packed together, and finally the line data were packed together. Adding, for instance, one additional ion to the existing data had required changes in many places of the standard input – the total number of levels was changed, the overall indexing of levels was changed, which required changes in practically all blocks of input. Also, it required a painstaking recalculating of the relation between absolute and relative level indices for the levels of the individual ions.

In contrast, the new system of input enables the user to set up a library of more or less universal data sets for all the astrophysically important ions, and to select a desired degree of sophistication of a model atmosphere easily by pointing to those filenames the standard (unit 5) input. Notice that the standard input only contains filenames of the input data for the individual ions, but no overall indexing is required. This is set up by the program.

Moreover, there is an IDL–based program called MODION, written by F. Varosi (NASA/GSFC), which is designed to construct the individual ionic input files directly from the Opacity Project (OP) database TOPBASE. The program displays the Grotrian diagram of a selected ion, and the user selects explicit levels, and/or build superlevels, simply by a mouse. Program MODION then

builds an array of bound-bound and bound-free transitions. For the latter, the user may form an approximate photoionization cross-section graphically from the detailed OP cross-sections. The "new" format of input to TLUSTY thus perfectly dovetails this new tool, but is very useful also for a user who does not use MODION.

Important note: Unlike the standard input (Unit 5), the ionic files *must not* contain "comment lines" beginning with * or !. Instead, there is one mandatory record beginning by * immediately preceding each block, i.e the structure of the file looks for instance as follows:

`****** Levels`

followed by data for energy levels, without any comment line,

`****** Continuum transitions`

followed by data for bound–free transitions, without any comment line,

`****** Line transitions`

followed by data for bound–bound transitions, without any comment line.

We will now describe the three basic blocks of the ionic input file in detail.

6.1 Energy level parameters

By the term "level" we mean here either a genuine atomic energy level, or any reasonably defined group of energy levels, e.g. a superlevel (see Hubeny and Lanz 1995). There are two types of superlevels:

i) a genuine superlevel, which is a pre-defined group of levels; all the input parameters have to be specified (used for instance for the iron-peak elements); and

ii) a "merged level", which is a superlevel composed of all merged Rydberg, partially dissolved, states of an ion. The level parameters, such as statistical weight and a mean energy, are considered as depth-dependent (because of a depth-dependent dissolution), and are computed by the program.

Each energy level has one input record containing the following parameters:

ENION – ionization energy of the level (with respect to the ground level of the next ionization
  state may be given either in erg, eV, cm^{-1}, or as frequency (s^{-1}).
  = 0 – the program assigns the hydrogenic ionization energy, assuming that the principal quantum number is the order number of level within the corresponding ion

G – statistical weight;
  = 0 – the program assigns the hydrogenic statistical weight, analogously as for level energies.

NQUANT - principal quantum number.
  =0 – the program assigns for NQUANT the serial number of the level;
  < 0 – indicates that the given level is kept in LTE (even if the model is NLTE); NQUANT is then set to abs(NQUANT)

TYPLEV – character*10 string – a spectroscopic identification of the level. It appears only in outputs, but may also be used as an identifier in the case of using the pretabulated photoionization cross-section data

IFWOP – an mode of the treatment of level dissolution (See Hubeny, Hummer, & Lanz 1994):

$= 0$ – occupation probability set to 1, i.e no level dissolution ;

> 0 – occupation probability of the level is calculated, and is used consistently in the rate equations and in evaluating the opacities and emissivities. The occupation probabilities are calculated in the hydrogenic approximation, i.e., they may be used for any atom/ion, but for non-hydrogenic ions they are of a limited accuracy.

< 0 – signals that the level is a so-called merged level (i.e. the Rydberg states lumped together).

FRODF – dummy (a former option, now obsolete), kept for downward compatibility of the input data.

IMODL – a mode of treating a linearization of the level population:

$= 0$ – explicit level – the population is linearized;

> 0 – the level population is solved for exactly in the formal solution step, but the population is not explicitly linearized. The actual treatment of the level population (e.g. its partial or implicit linearization) is determined by the actual value of IMODL.

< 0 – the level population is not solved for exactly in the formal solution step, neither it is explicitly linearized. The actual treatment of the level population is determined by the actual value of IMODL.

$= 1$ – updated b-factor – the b-factor is fixed in the linearization, and is updated in the formal solution;

$=-1$ – fixed b-factor – the b-factor is fixed and is never updated;

$= 2$ – updated population – the population is held fixed in the linearization, and is updated in the formal solution;

$=-2$ – fixed population – the population is fixed and is never updated. $= 5$ – updated generalized b-factor – the generalized b-factor is fixed in the linearization, and is updated in the formal solution; the generalized b-factor is defined is a ratio of the actual population to the population which is in LTE with respect to the reference level (not necessarily the ground state of the next ion);

$=-5$ – fixed generalized b-factor – the generalized b-factor is fixed and is never updated;

$= 6$ – updated population ratio – the ratio of the population to the reference level population is held fixed in the linearization, and is updated in the formal solution;

$= -6$ – fixed population ratio – the ratio of the population to the reference level population is held fixed and is never updated.

Note: The mode IMODL is introduced for two different purposes. First, one needs fully fixed populations (say of hydrogen and helium) for evaluating the so-called "background opacities" in the case when temperature and density is held fixed, and one only solves a coupled radiative transfer and statistical equilibrium for a selected atom or several atoms (mode IMODL=−2). Second, by not linearizing populations of some levels, but rather only updating the populations in the formal solution, one may speed up the calculation, and in some cases prevent convergence problems (options IMODL= 1, 2, 5, 6). In most cases, options 5 and 6 give the best results. We stress again that the switch IMODL may be globally overwritten by coding parameter IFLEV to be non-zero.

6.2 Parameters for bound–free transitions

The structure is as follows. Each transition which is to be taken into account is specified by one standard record. If the transition is assumed to be in detailed radiative balance, there are no other records. Otherwise, there are one or more additional records for each transition, depending on the actual values of some control parameters.

The standard record of input parameters for continuum transitions

II – index of the lower level

JJ – index of the upper level

MODE – mode of treating treating the radiative rates in the transition:
> = 0 – detailed radiative balance (i.e. radiative rates are not evaluated; but collisional rates are);
> > 0 – primarily linearized transition;
> < 0 – primarily ALI transition;
> Note: the distinction "primarily linearized" or "primarily ALI" does not have any meaning for continua;
> abs(MODE) = 5 or 15 – signals that the given continuum is supplemented by a pseudo-continuum. Pseudocontinuum is a dissolved part of a corresponding spectral series converging to the given edge. In this case, there is one additional record immediately following the present one, which specifies the minimum frequency to which the pseudo-continuum is considered.

IFANCY – a mode of evaluation of the photoionization cross-section (for detailed expression, see Appendix):
> = 0 – hydrogenic photoionization cross-section, with Gaunt factor set to 1;
> = 1 – hydrogenic cross-section with the exact Gaunt factor;
> = 2 – cross-section by a Peach-type expression;
> = 3 – modified Peach-type expression (called Henry-type);
> = 4 – Butler's fit formula (polynomial fits to the Opacity Project results);
> = 5 – cross-section from Verner tables;
> = 7 – hydrogenic cross-section with the Gaunt factors from Klaus Werner;
> = 9 – Opacity Project data stored in a special file, named RBF.DAT (obsolete option)
> = 11 or 13 – Opacity Project cross section for He I with Seaton-Ferney's cubic fits;
> = 11 – means that the multiplicity S=1 (singlet);
> = 13 – means that the multiplicity S=3 (triplet);
> = 10 – cross section for He I, based on Opacity Project, but appropriately averaged for an averaged level (see explanation in SBFHE1);
> = 21 – Cross-section for ground state of He I from Koester fit (A&A 149, 423);
> > 49 and < 100 – special cross-section for a superlevel, precalculated. IFANCY then indicates the input unit number from which the data are read.
> > 100 – Opacity Project data, immediately following the given record. There are IFANCY − 100 data points.
> < 0 – non-standard expression, given by a user supplied subroutine (SPSIGK).

ICOL – mode of evaluation of the collisional rate:
> ≥ 0 – means that collisional rate is evaluated by some standard expression, already coded in the program – see Appendix for details.

= 0 – Seaton's formula. Here the value of the photo-ionization cross section at the threshold is transmitted in array OSC0;

= 1 – Allen's formula; again, OSC0 has the meaning of the necessary multiplicative parameter;

= 2 – the so-called SIMPLE1 mode - see Appendix;

= 3 – the so-called SIMPLE2 mode - see Appendix;

< 0 – non-standard expression, given by a user–supplied procedure (CSPEC)

IFRQ0, IFRQ1 – a means of setting some frequency points in the continuum to the linearized mode in the case of automatic setting of frequency points. Notice that in such a case the continuum frequency points are treated by default in the ALI mode. If IFRQ0 and IFRQ1 are non-zero, then all the frequency points between the IFRQ0-th and IFRQ1-th point in the continuum are set to linearization mode. Typically, one sets IFRQ0=1 and IFRQ1=4 for the hydrogen Lyman continuum, and sometimes analogously for the He II Lyman continuum.

OSC0 – first collision parameter (see Appendix for details);

CPARAM – second collision parameter (see Appendix for details).

Additional input parameters for continuum transitions

In most cases, there is one or more additional input records for the continuum transition, which depends on coded values of the basic parameters listed in the first record, described above.

• (1) For MODE = 5 or 15, i.e. when the given continuum is supplemented by a pseudo-continuum (i.e. a dissolved part of a corresponding spectral series converging to the given edge. In this case, there is one additional record immediately following the present one, containing one number:

FR0PC – the minimum frequency to which the pseudo-continuum is considered.

• (2) For IFANCY = 2, 3, or 4, there is one additional record containing 4 numbers:

S0, ALF, BET, GAM – parameters for evaluation the photoionization cross-section in the Peach, Henry, and Butler form. See Appendix for the detailed meaning of these parameters in each individual case.

• (3) For IFANCY > 100, there are two or more additional records, containing the fit points for the Opacity Project photo-ionization data. The actual value of IFANCY has the meaning that there are IFANCY−100 fit points. The first (or more, if needed) record(s) then contains IFANCY−100 values of XTOP, followed by the same number of records with values of CTOP, where

XTOP – the value of x, $x = \log_{10}(\nu/\nu_0)$, of a fit point, where ν_0 is the edge frequency;

CTOP – the corresponding value of the cross-section, expressed as CTOP $= \log_{10}(\sigma_\nu \times 10^{18})$ of a fit point.

6.3   Parameters for bound-bound transitions

The structure is analogous to that for the bound-free transitions, § **??**. Each transition which is to be taken into account is specified by one standard record. If the transition is assumed to be in detailed radiative balance, there are no other records. Otherwise, there are one or more additional records for each transition, depending on the actual values of some control parameters.

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The standard record of input parameters for line transitions

II – index of the lower level

JJ – index of the upper level

MODE – mode of treating treating the radiative rates in the transition.

= 0 – detailed radiative balance (ie. radiative rates are not evaluated; but collisional rates are);

> 0 – primarily linearized transition;

< 0 – primarily ALI transition;

= 1 or −1 – a "normal" line (i.e any line not represented by an ODF);

= 2 or −2 – an ODF corresponding to the transition from a normal to a "merged" level (i.e. all high members of a spectral series lumped together). In this case, the ODF is calculated by TLUSTY. This option is typically used for H and He II.

= 3 or −3 – a "normal" ODF, representing a superline – a transition between two normal superlevels. The ODF is calculated by a separate program, and is communicated to TLUSTY by means of two additional input files (see § **??**).

= 9 or −9 – a contribution of the transition to the total radiation pressure is set to zero. This option represents a means of avoiding numerical as well as physical instabilities in the atmosphere due to a large radiation pressure in certain individual strong lines (like C IV or N V resonance lines).

> 100 or < −100 – the next immediate input record contains frequency or wavelength of the transition; MODE is immediately changed to MODE−100 (or MODE+100 for negative MODE). This option is useful if one needs a different frequency of the transition than that corresponding to a difference of level energies (for instance for avoiding an overlap of a normal and an ODF line).

IFANCY – a mode of treatment of the absorption profile (has the meaning for the "normal" lines only, i.e. with abs(MODE)=1:

= 0 – Doppler profile;

= 1 or −1 – Voigt profile;

= 2 or −2 – Stark (+ Doppler) profile for hydrogenic lines;

≥ 10 – non-standard expression, given by a user-supplied subroutine (PROFSP);

> 0 – the absorption profile for the farthermost frequency point(s) from the line center is(are) taken to be 0;

< 0 – the absorption profile for the farthermost frequency point(s) evaluated exactly.

ICOL - mode of evaluating collisional rates:

≥ 0 – means that collisional rate is evaluated by some standard expression, already coded in the program – for details see Appendix.

< 0 – non-standard expression, given by a user–supplied procedure (CSPEC);

= 0 – Van Regemorter formula, with a "standard" $\bar{g} = 0.25$

= 1 – Van Regemorter formula, with an "exact" $\bar{g}$; $\bar{g}$ is transmitted in CPAR;

= 2 – the so-called SIMPLE1 mode - see Appendix;

= 3 – the so-called SIMPLE2 mode - see Appendix;

= 4 – Eissner-Seaton formula - see Appendix;

The meaning of ICOL for is different for H, He I and He II:

• ICOL = 0 – approximate expressions taken from Mihalas, Heasley and Auer (1975);

For He I bound-bound transitions, the following standard possibilities are also available:

• ICOL = 1, 2, or 3 – much more accurate Storey's rates, subroutine written by D.G.Hummer (COLLHE). This procedure can be used only for transitions between states with $n = 1, \ldots 4$.
• ICOL = 1 – means that a given transition is a transition between non-averaged ls states. In this case, labeling of the He I energy levels must agree with that given in subroutine COLLHE, ie. states have to be labeled sequentially in order of increasing frequency.
• ICOL = 2 – means that a given transition is a transition between a non-averaged ls lower state and an averaged upper state.
• ICOL = 3 – means that a given transition is a transition between two averaged states.

IFRQ0, IFRQ1 – their non-zero values signal a change for the mode of treatment frequency points (i.e. ALI or linearized) between indices IFRQ0 and IFRQ1 (internal indices for a line, starting with 1). For instance, if the given transition is primarily an ALI one (MODE<0), then the points between IFRQ0 and IFRQ1 will be taken as linearized.

OSC – oscillator strength
= 0 – the program assigns a scaled hydrogenic oscillator strength;

CPARAM – second collision parameter (see Appendix for details)

Additional input parameters for line transitions

In most cases, there is one or more additional input records for the line transition, which depends on coded values of the basic parameters listed in the first record, described above. In case there are more input records, they should appear in the order in which they are listed below:

(1) modified frequency of the line – if abs(MODE) > 100.

FR0INP – frequency (or wavelength – if FR0INP < 10^{10} the value is understood as wavelength in Å) of the line, if it is required to be different from the value computed from the corresponding level energies. This option is useful, for instance, for avoiding a spurious overlap of a normal and an ODF line.

(2) Additional input parameters for "normal" line transitions, i.e. those not represented by ODF's – with abs(MODE)=1.

LCOMP – a mode of considering the absorption profile:
= .FALSE. – depth-independent profile;
= .TRUE. – depth-dependent profile.

INTMOD – a mode of setting the frequency points and weights in the line:
= 0 – means that frequency points and weights have already been read amongst the NJREAD or NFREAD frequencies; $\neq 0$ – frequency points and weights are evaluated, with one of the following possibilities:
= 1 – equidistant frequencies, trapezoidal integration;
= 2 – equidistant frequencies, Simpson integration;
= 3 – a "modified Simpson" integration, which is a set of 3-point Simpson integrations with each subsequent integration interval doubled, until the whole integration area is covered;
= 4 – frequencies (in units of standard x; x being the frequency displacement from the line center measured in units of fiducial Doppler width) and weights (for integration over x) are read from the record(s) immediately following.

NF – number of frequency points in the line (has the meaning only for INTMOD $\neq 0$)

XMAX – the maximum frequency extent of the line (in units of fiducial Doppler width):
   $= 0$ – program sets up default XMAX=4.55
   > 0 – means that the line is assumed symmetric around the center; the frequency points are set up between $x = 0$ and $x =$ XMAX, where x is frequency difference from the line center in units of the fiducial Doppler width (the fiducial Doppler width is the Doppler width calculated with the standard temperature TSTD and the standard microturbulent velocity VTB);
   < 0 – frequency points are set between $x =$ XMAX and $x = -$XMAX
   Important note: in the overlapping mode (IOVER > 0), all lines are set by default to the full-profile mode. Thefore, even if XMAX was coded as positive, it is reset to $-$XMAX, and NF is reset to $2 \times$ NF $- 1$.

TSTD – characteristic temperature for evaluating the fiducial Doppler width:
   $= 0$ – the program sets the default standard temperature, TSTD $= (3/4) \, T_{\text{eff}}$

(3) If a Voigt profile is assumed (ie. if IPROF $= 1$), an additional input record is required which specifies an evaluation of the relevant damping parameter – see subroutine DOPGAM)

GAMR – a natural broadening indicator:
   > 0 – has the meaning of natural damping parameter (i.e. the Einstein coefficient for spontaneous emission);
   $= 0$ – classical natural damping assumed $\Gamma = 2.4734 \times 10^{-8} \, \nu^2$;
   < 0 – natural damping is given by a non-standard, user supplied procedure GAMSP

STARK1 – Stark broadening indicator:
   $= 0$ – Stark broadening neglected;
   < 0 – scaled classical expression, i.e. $\Gamma = -$STARK1 $\times \Gamma^{\text{clas}}$, where $\Gamma^{\text{clas}} = 10^{-8} \, n_{\text{eff}}^{5/2} \, n_{\text{e}}$, where n_{eff} is the effective quantum number of the upper level;
   > 0 – Stark broadening given by $n_{\text{e}} \, (\texttt{STARK1} \times T^{\texttt{STARK2}} + \texttt{STARK3})$, where $\texttt{STARK2, STARK3}$ are the input parameters

STARK2, STARK3 – see above;

VDWH – Van der Waals broadening indicator:
   ≤ 0 – Van der Waals broadening neglected;
   > 0 – a scaled classical expression.

(4) Additional input parameters for a "merged superline" transition, i.e. a transition to a merged level, treated by means of an ODF – i.e. for abs(MODE)=2:

KDO(1),KDO(2),KDO(3),XDO(1),XDO(2),XDO(3),KDO(4) – the parameters which have the following meaning: The superline is represented by four frequency intervals. Going away from the peak of ODF, the first interval is represented by a KDO(1)–point Simpson integration, with a distance XDO(1) fiducial Doppler widths between the points. The same for the second and third interval. The rest (the interval between the last point and the corresponding edge) is represented by a KDO(4)-point Simpson integration. The fiducial Doppler width is that corresponding to the effective temperature.

6.4 Examples

Energy levels

An input for hydrogen is very simple; for instance the ground state is specified by the following record

```
0.                    0.   0     ' (N=1) '   1     0.    0
```

because the energies and statistical weights are hydrogenic. The number 1 in the fifth entry signifies that the exact occupation probability and level dissolution will be taken into account. The "merged" level is specified by

```
0.                    0.   0     ' merged '  -1    0.    0
```

The He I ground state is specified by

```
5.94503520D+15        1.   1     '1 sing S'  0     0.    0
```

Bound-free transitions

The hydrogen Lyman continuum, for a hydrogen model atom composed of 9 levels for H I and one level for H II, is specified, for instance, by

```
1 10  5  1  0  1  4  0.  0.     ! Lyman continuum supplemented by pseudocontinuum
2.6D15                          ! Lyman pseudocontinuum extends to nu=2.6D+15
```

The 6-th and 7-th entry, IFRQ0 and IFRQ1, signify that the 1st through 4th frequency points in the Lyman continuum (the points immediately blueward of the discontinuity) will be treated in the linearized (not ALI) mode. As mentioned earlier, this option is usually a recommended one, since it usually increases the convergence rate considerably, while the total computer time remains virtually unchanged (see also an extensive discussion in Hubeny & Lanz 1995).

Another example is a specification of the ground state of N III, viz

```
  1  16   1    107     0      0      0   5.006E-19   0.000E+00
  0.002  0.024  0.069  0.169  0.550  0.928  1.170
  0.232  0.359  0.401  0.232 -0.528 -1.384 -2.113
```

which shows how to use a fit point representation of the OP photoionization data. In this case, there are 7 points (IFANCY=107), with relative frequencies x specified in the second record, and the logarithms of cross-sections (in mB) in the third. Other features: the collisional rate is evaluated by the Seaton formula (ICOL=0 – the 5th entry in the first record), with the parameter $\sigma_0 = 5.005 \times 10^{-19}$ – the 8th entry.

Line transitions

The hydrogen Lα line is specified, for instance, by

```
1   2  -1    0  0  6  8  0.  0.
 F   1  7  0.  0.
```

In this case, the line frequencies are predominantly taken in the ALI mode (MODE=−1), but points 6 − 8 are set to a different treatment, i.e. are linearized. The line is taken with a depth-independent (LCOMP=F), Doppler profile (IFANCY=0). The number of frequency points is set to 7 (NF=7), but we assume the standard value of the line-overlap mode switch IOVER=1, in which case the line is automatically taken with full profile (extending to both sides from the line core), with the actual number of frequency points being $2 \times 7 - 1$, i.e. 13.

Analogous input for Lα, but with full (depth-dependent) Doppler + Stark broadening, is for instance

```
  1   2 -1    2   0 22 32  0.  0.
T 3  27  1022 0.
```

where the line is assumed to extend to 1022 fiducial Doppler widths, and the line is represented by 53 frequency points.

If Lα is assumed to be in detailed radiative balance, one codes a single record,

```
  1  2  0  0  0  0  0  0.  0.
```

We stress that there is a significant difference between specifying the mode of treating Lα as above, and not specifying the transition at all. In the later case, neither collisional, not radiative rates are calculated, i.e. the transition is assumed to be in both radiative and collisional detailed balance. The levels are thus forced to be in exact Boltzmann equilibrium within each other. In the former case, the collisional rates are calculated, but the levels are not forced to be in equilibrium. Departures from equilibrium are determined by relative values of the collisional rates and respective photoionization rates.

7   STANDARD INPUT IN THE "OLD" FORMAT

The old system of input was extensively described in the User's Guides for the previous versions. Since the program evolved significantly in between, not all of the input parameters which version 195 accepts are described there. The old format of input has to specify all the standard, non-standard, and ionic parameters described in the previous three sections. Since the meaning of all parameters was explained there, we will only give here the actual READ statements form the program (subroutine START0). This way, we show the order in which the parameters are read, but will not repeat the explanation, unless the meaning of a parameter is somewhat different between the "new" and "old" formats of input.

As discussed in the previous Guides, the "old" standard input file (Unit 5) is organized into 8 basic blocks; each block being generally composed of several records. The actual number of records in a block depends on actual values of certain parameters read previously (as, for instance, on the number of explicit atoms, ions, levels, transitions, etc.). Also, in some cases, setting certain flags to negative values implies reading one or more additional input records which would otherwise be absent. If not read from the standard input, such "hidden" input parameters attain their default values.

The eight constituent blocks of the standard input are the following:

1. Basic input parameters

2. Frequency points

3. Turbulent velocity

4. Input parameters for individual explicit and implicit atoms

5. Input parameters for individual explicit ions

6. Input parameters for individual explicit levels

7. Input parameters for individual transitions

8. Additional parameters

The last block is a very heterogeneous mixture of both physical parameters and performance flags. Also, while the structure of the first seven blocks is quite regular, the structure of the last block depends to a large extent on input data.

  We now turn to a description of the individual input parameters. We will show the way the program reads the input data by a pseudocode, which is exactly parallel to the actual FORTRAN code (a part of subroutines START0 and STATE, which read the input data. We use the form of a pseudo-code for a shorter and more comprehensible description of the input.

First block − Basic Parameters

The block is composed of 3 records (or more, depending on the values of flags IFALI, IATREF, and IRTE).

```
    READ TEFF,GRAV,HMIX0
    READ LTE,LTGREY,LCHC,ISPLIN,CHMAX
    IF(ISPLIN.LT.0) THEN
        reset ISPLIN (to -ISPLIN if IPLSIN.lt.-5 or else to 0)
        READ IBC,IRDER,ILMCOR,ILPSCT,ILASCT,IRTE,IDLTE
        IF(IRTE.GE.2) THEN
            READ DJMAX,NTRALI
        END IF
    END IF

    READ NITER,ND,NATOM,NION,NLEVEL,IFALI,IFPOPR,IATREF,NELSC
    IF(IFALI.GT.10) THEN
        reset IFALI to IFALI-10
        READ IFPREC,IOVER,ITLAS,IELCOR,IHECOR
        READ IACCP,IACDP
        READ ILDER,IBPOPE,CHMAXT,NLAMT
    END IF
```

In case the parameters IBC, IRDER, etc, are not read (i.e. if ISPLIN is coded as positive, etc., the program assumes default values, which are exactly the same as defaults for the "new" format of input.

  The parameters not explained in the previous sections, or those with a different meaning, are explained below:

TEFF − effective temperature;
    < 0 − has to be coded if an external irradiation is allowed for; TEFF is reset to $-$TEFF.

GRAV – $\log g$

    < 0 – means setting INTRPL$= -1$, i.e. assuming the starting model atmosphere to by a Kurucz model; GRAV is reset to abs(GRAV)

LCHC – a logical equivalent of ICHC (§ **??**), LCHC = ICHC.EQ.1

NATOM – total number of explicit atoms;

    < 0 – parameter IBFINT is set to 0 (which means that photoionization cross-sections are stored for all frequencies - see § **??**); NATOM is reset to abs(NATOM)

NION – total number of explicit ions, not counting the highest ionization degrees of the species

NLEVEL – total number of explicit levels;

    < 0 – parameter IRSPLT is set to 1, which indicates that the rate matrix is not inverted as a whole; instead, one solves several separate sets of statistical equilibrium equations (with partial rate matrices) for each individual species – see § **??**. Notice that the default in the "old" input is IRSPLT=0! This is one of very few differences in default values between the "new" and "old" inputs.

IFALI – have the same meaning as in § **??** for positive values, plus JALI is set to 1 (Rybicki-Hummer algorithm for evaluating Λ^*);

    < 0 – sets JALI=2, i.e. the Olson-Kunasz Λ^*; IFALI is reset to abs(IFALI)

IATREF – a reference level indicator – see § **??**:

    $= 0$ – sets IATREF=1 and MODREF=0;
    > 0 – sets MODREF=1;
    > 100 – sets IATREF to IATREF-100 and MODREF=2;
    < 0 and > -100 – sets IATREF=$-$IATREF and MODREF=0;
    < -100 – sets IATREF to $-$IATREF-100 and MODERF$= -1$; plus the reference levels for each explicit atom, NREF(IAT), IAT=1,NATOM are read from the subsequent record(s).

Second block − Frequency Points

The structure of this block is analogous to the block of Frequency points, described in § 4.2. There is one record containing NJREAD, and then depending on whether NJREAD is positive or negative, either one additional record (for an automatic setting of frequency points), or NJREAD records with data for the individual points. Finally, there is one additional record at the end of this block.
Important note: The meaning of NJREAD is reversed with respect to the analogous parameter NFREAD of the new input.
• If NJREAD > 0, the program assumes explicit input of frequencies, in which case there are NJREAD records, exactly the same as in the new format.
• If NJREAD < 0, the program assumes an automatic setting of frequencies, and the next record contains. The block is read as follows

```
    READ NJREAD
    IF(NJREAD.LT.) THEN
       reset NJREAD to -NJREAD
       READ FRCMAX,FRCMIN,FRLMAX,FRLMIN
     ELSE
       DO IJ=1,NJREAD
          READ FREQ(IJ),W(IJ),WCH(IJ),IJALI(IJ)
```

```
        END DO
    END IF
    READ NFFIX,IFSUB,IFLEV
        reset IFLEV
        READ POPZER
    END IF
```

Here, parameter NFFIX is identical to IFRALI (§ **??**).

Notes:

- There is a separate program SETFRE which generates the above described input for the continuum frequency points. This program is a part of the package. However, since version 195 is able to produce the frequency points automatically, program SETFRE is somewhat obsolete.

- Although the frequency points read in this block are referred to as "continuum" frequency points, they may also describe some selected lines. If a line has a full set of points already specified withing the NFREQC frequencies, the corresponding input for this line should be set in such a way that the frequency points for this line will no set up again. However, we stress again that in the overwhelming majority of uses of the program, the frequency points discussed above should be selected to cover only the continua; the frequency points in lines are usually set up by the program (see the seventh block). This is usually a highly recommendable option.

- If the frequency points are set up manually, it must be kept in mind that the frequency points in continua *must* be ordered by decreasing frequencies. The frequency points in individual spectral lines (usually set up by the program) may then be ordered quite arbitrarily.

- We stress again that there is no universal recipe to chose which frequency points are linearized. An optimum choice can be found with an extensive experimentation, which is almost never worth it. The most reasonable strategy is simply to set a few (2-4) frequency points in a few (1 - 3) most opaque continua (this points immediately shortward of the edges) to be linearized. In some cases, it is not necessary to select any point to be linearized.

Third block – Turbulent Velocity

This block usually contains just one record, but may contain more if a depth-dependent turbulent velocity is assumed.

```
    READ ITB,VTB
    IF(ITB.NE.0) THEN
        READ (VTURB(ID),ID=1,ND)
    END IF
```

In other words, VTB has the same meaning as above; ITB signals that a depth-dependent turbulent velocity is assumed; following records contain the corresponding values. The depth-dependent turbulent velocity input is not supported by the "new" format of input, but may be easily reintroduced if required. (The option was dropped because it was never used in any application of TLUSTY so far.) Again, values of VTB or VTURB are either in km s^{-1} (if numerically smaller than 10^3), or in cm s^{-1}.

Note: Microturbulent velocity is allowed to contribute both to the line broadening (via modifying the Doppler widths), as well as to the hydrostatic equilibrium via the turbulent pressure.

Fourth block - Atoms

This block is read by subroutine STATE. The block contains one input record with a value of NATOMS, and then NATOMS analogous records.

```
READ NATOMS
DO I=1,NATOMS
    READ MA,NAO,NAK,ION,MODPF,ABN
    IF(ABN.GT.1.E6) READ (ABNDD(I,ID),ID=1,ND)
END DO
```

Here, NATOMS, MODPF(I), and ABN have the same meaning as the analogous quantities of the "new" input format (see § 4.3), MA is the same as MODE there. The additional parameters for the "old" input format:

NA0, NAK – have the meaning only for MA=2, and indicate that the explicit energy levels of the present species have the indices between NA0 and NAK (NAK is thus the index of the highest ionization state, which is represented by a one-level ion).

ION – has the meaning for MA=1 only;
= 0 – the default number of ionization degrees is considered;
> 0 – then ION ionization degrees is considered (counting also the neutrals).

The same conventions and limitations as those described in § ?? apply here as well.

Fifth block − Ions

This block contains NION (see the First block) analogous records, viz.

```
DO I=1,NION
    READ NFIRST(I),NLAST(I),NNEXT(I),IZ(I),IUPSUM(I),
*           ICUP(I),MODEFF,NFF,TYPION(I)
    IF(NFIRST(I).LT.0) THEN
        reset NFIRST(i) to -NFIRST(I)
        READ INODF1(I),INODF2(I)
    END IF
END DO
```

where the parameters IUPSUM,ICUP,MODEFF,NFF,TYPION,INODF1,INODF2 were described in § ?? and ??. The additional parameters needed here have the following meaning:

NFIRST – index of the first explicit level of the ion;
< 0 – indicates that for the given ion one has a precalculated set of ODF's (opacity distribution functions). In this case, there is an additional record indicating two unit numbers where the ODF input is going to be read from (called INODF1(I) and INODF2(I); NFIRST is then set to abs(NFIRST)

NLAST – index of the last explicit level of the ion

NNEXT – index of the ground state of the next higher ionization state;
< 0 - indicates that the given ion will be treated in LTE (even if the current model is NLTE). NNEXT is then set to ABS(NNEXT)

IZ(I) – effective charge (= 1 for neutrals, 2 for once ionized, etc.)

Sixth block – Levels

The structure of the block is exactly the same as in the case of the "new" format described in § ??, only here are data for all energy levels of all atoms and ions packed together. The order of input records for individual levels is important, because it determines the *index* of the level. There must not be a conflict between the indexing of levels defined this way, and the parameters N0A, NKA; and NFIRST, NLAST, NNEXT from the previous two blocks.

Seventh block – Transitions

Again, the structure of the block is exactly the same as in the case of the "new" format described in § 6.2 and § 6.3. The only difference here is that data for all transitions of all atoms and ions packed together. The particular order in which the input data for the individual transitions occur does not matter; the transitions may be ordered my species, or first all continuum transitions and then all the line transitions (the usual option). However, if the level indices are not coded as absolute indices, then it is safer to order the transitions by species.

   Although the meaning of the input parameters is generally the same as that described in § ?? and ??, parameters II and JJ (from the basic input record for a transition) may now have a special meaning.

II and **JJ** – are the indices of the lower and upper level of the transition, respectively. These indices may be coded in two different ways:

1. as the "absolute" index, i.e. a level has an index corresponding to the global numbering of all levels considered (see also previous input block).

2. as a "relative" index (i.e. starting from II=1 for each ion; for instance to be able to code for Lα II=1, JJ=2, regardless of the absolute indices of levels, which may obviously be different from 1 and 2, respectively). This is achieved by putting a record with II=0 and JJ=JJ0 > 0 (subsequent parameters having no meaning); which signals that in all the subsequent input (until an analogous records is met); the input values of II and JJ have the meaning of relative indices, JJ0 being the reference index (offset); ie. the absolute indices are II+JJ0−1 and JJ+J0−1.

A record with **both** II and JJ equal to 0 signals the end of input data for atomic transitions.

Eighth block – Additional Parameters

This is very heterogeneous block. All the parameters which are explicitly read here are the "non-standard" parameters in the terminology of the "new" input format. In the "old" format, the block is rather cumbersome.

   The block is read is follows:

```
READ IOPADD
IF(IOPADD.GT.0) READ IRSCT,IOPHMI,IOPH2P,IOPHE1,IOPHE2

IF(.NOT.LTGREY) THEN
   READ INTRPL,ICHANG
 ELSE
   READ NDEPTH,TAUFIR,TAULAS,ABROSO,TSURF,ALBAVE,DIONO
   READ IDEPTH,NCONIT,IPRING,IHM,IH2,IH2P
```

```
      END IF

      READ NLAMBD
      IF(NLAMBD.GT.0) THEN
         DO I=1,NLAMBD
            READ IDUMMY
            READ IDUMMY
         END DO
       ELSE IF(NLAMBD.LT.0) THEN
         NLAMBD=-NLAMBD
      END IF

      READ ICLMAT,ICONV,IPRESS,ITEMP,IPRINT
      IF(ICLMAT.NE.0) THEN
         READ INHE,INRE,INPC,INSE,INMP,INDL,NDRE,TAUDIV,IDLST
         READ DUMMY
      END IF

      READ IACC,IACD,ORELAX,ITEK
      IF(ITEK.LT.0) READ (KANT(I),I=1,NITER)

      READ IWINBL
      IF(IWINBL.EQ.-1) THEN
         READ TRAD,WDIL
       ELSE IF(IWINBL.LT.-1) THEN
         READ (EXTRAD(IJ),IJ=1,NFREQ)
      END IF

      READ NPGPOP
      READ ICRSW,SWPFAC,SWPLIM,SWPINC
```

Notes:
• To recover default values listed in Chapter 5, one has to code the block, for a NLTE model, as

```
 0                    ! IOPADD
 0  0                 ! INTRPL,ICHANG
-1                    ! NLAMBD
 0  0  0  0  0        ! ICLMAT,ICONV,IPRESS,ITEM,IPRINT
 7  4  0  5           ! IACC,IACD,ORELAX,ITEK
 0                    ! IWINBL
 0                    ! NPGPOP
 0  0  0  0           ! ICRSW,SWPFAC,SWPLIM,SWPINC
```

or, for an LTE model, starting with LTE-gray (i.e. LTGRAY=.TRUE.), as

```
 0                        ! IOPADD
 70 1.D-7 3.16D2 0.4  0  0  1. ! LTE-GRAY INPUT1
 0  0  0  0  0  0      ! IDEPTH,NCONIT,IPRING,IHM,IH2,IH2P
-1                        ! NLAMBD
```

```
0  0  0  0  0          ! ICLMAT,ICONV,IPRESS,ITEMP,IPRINT
7  4  0  5             ! IACC,IACD,ORELAX,ITEK
0                      ! IWINBL
0                      ! NPGPOP
0  0  0  0             ! ICRSW,SWPFAC,SWPLIM,SWPINC
```

• Parameter NLAMBD, if coded positive, is followed by $2 \times$ NLAMBD dummy input records. This is a leftover from previous version, and this format of input is kept for downward compatibility of old input data sets. To simplify the input, coding negative NLAMBD avoids this unnecessary input.

• Coding ITEK as negative switches on an additional input of parameters **KANT** (for all global iterations ITER=1,NITER), where

KANT=0 – signifies a full linearization iteration;

KANT=1 – a Kantorovich iteration (i.e. no new Jacobi matrix of the linearized equations is set up and inverted).

• Wind blanketing is included only for historical purposes. If it is not considered (the usual option), this sub-block consists of only one record with single zero. If it is to be considered, there are several other input records; the user is encouraged to consult the listing of the program. Notice also that the input for external irradiation is read if IWINBL is coded negative.

8   STARTING MODEL ATMOSPHERE

Except computing an LTE model from scratch (i.e. LTE-gray model, by coding `LTGRAY = .TRUE.`, a starting model atmosphere is needed. It is transmitted by input Unit 8. In most applications, the user does not have to care about the structure of the file because it is usually created by a previous run of TLUSTY.

However, the program also accepts model atmosphere created by TLUSTY with different choice of explicit atoms, ions, and energy levels than that which is specified for the current run. This is straightforward if the starting model is an LTE one, because the only transmitted model parameters are temperature, electron density, and mass density. However, if the starting model is an NLTE one, the input also contains all the explicit level populations, and therefore would be incompatible with the current indexing of levels. Consequently, a special input is needed in these cases, which is signaled by coding the parameter ICHANG to be non-zero.

Finally, the program accepts as a starting model a Kurucz model atmosphere in Kurucz's standard format. We will now describe the relevant input parameters in detail.

8.1   TLUSTY input model atmosphere

• **1st line**:

NDEPTH – number of depth points in which the initial model is given (if not equal to ND, routine automatically interpolates to the set DM by linear interpolation in log(DM).

NUMPAR – number of input model parameters in each depth:
     = 3 – for LTE model;
     > 3 – for NLTE model

• **Next block**:

DEPTH (ID=1,NDEPTH) – depth grid for the input model (i.e. a column mass in g cm^{-2})

• **For each depth point**:

T – temperature, T [K]

ANE – electron density, n_e (cm^{-3})

RHO – mass density, ρ (g cm^{-3})

level populations – only for NLTE input model. Number of input level populations need not
 be equal to NLEVEL; in that case ICHANGE should be coded as non-zero. Consequently,
 subroutine CHANGE is called from START to calculate the remaining level populations,
 and/or to change the indexing of levels – see below.

• If INTRPL > 0 – there is an additional input from unit 8, namely new depth scale DM (i.e. a
column mass in g cm^{-2}) which will be used in the current run.

8.2 Change of the input level structure

The change of the explicit level structure is controlled by parameter ICHANG – see § **??**. If this
parameter is coded positive, then the additional input, which specifies the correspondence of the
"old" (i.e. the input model) level populations and the 'new" ones (i.e. those which are to be
computed in the current run), is required. Generally, this option is useful, for instance, for adding
more explicit levels to an already converged model, without a necessity to start again from the
scratch.

For each explicit level in the "new" level population system, II=1,NLEVEL, the following
parameters are required:

IOLD – basic correspondence indicator:
 > 0 – means that population of this level is contained in the set of input populations; IOLD
 is then its index in the "old" (i.e. input) numbering. All the subsequent parameters have no
 meaning in this case.
 = 0 – means that this level has no equivalent in the set of "old" levels. An initial estimate
 of the population of this level has thus to be computed, following the specifications based on
 the following parameters:

MODE – indicates how the population is evaluated:
 = 0 – population is equal to the population of the "old" level with index ISIOLD, multiplied
 by REL;
 = 1 – the level is assumed to be in LTE with respect to the first state of the next ionization
 degree whose population must be contained in the set of "old" (ie. input) populations, with
 index NXTOLD in the "old" numbering. The population determined of this way may further
 be multiplied by REL.
 = 2 – population is determined assuming that the b-factor (defined as the ratio between the
 NLTE and LTE population) is the same as the b-factor of the level ISINEW (in the present
 numbering). The level ISINEW must have the equivalent in the "old" set; its index in the
 "old" set is ISIOLD, and the index of the first state of the next ionization degree, in the "old"
 numbering, is NXTSIO. The population determined of this way may further be multiplied by

REL.

= 3 – level corresponds to an ion or atom which was not explicit in the old system; population is assumed to be an LTE one.

NXTOLD – see above

ISINEW – see above

ISIOLD – see above

NXTSIO – see above

REL – a population multiplier – see above
   = 0 – the program sets REL=1

8.3   Kurucz input model atmosphere

TLUSTY also accepts Kurucz model as a starting model. The format of the file is the standard Kurucz output file. The Kurucz model is read is the parameter INTRPL is set to -1 (in the "new" input format), or parameter GRAV with a negative value (which is mandatory in the "old" input format.

One may still interpolate to a different depth grid than that used by Kurucz. Since parameter INTRPL cannot be used for this purpose, the user has to append internal INTRPL at the end of the Kurucz model file, followed by the values of m (g cm^{-2}).
Note: The first depth point of Kurucz models is usually incorrect, and is therefore skipped. If the user does not want to interpolate in depth, non-standard parameter ND should be set to 63 (i.e. ND=63 should appear in the non-standard parameter file (see § **??**).

9   OUTPUT

There are several output files. We divide them into two groups, listed and described below. By default, all the output files are generated as ASCII files for portability.

1. Basic output

   - Unit 6 – Standard output
   - Unit 7 – Condensed model atmosphere
   - Unit 9 – Convergence log
   - Unit 10 – Performance and error log
   - Unit 18 – Convergence log for formal solution
   - Unit 69 – Timing (Unix only)

2. Auxiliary output -

   - Unit 13 – Emergent flux in fixed and explicit frequency points
   - Unit 16 – Check of the statistical equilibrium equation solution

9.1 Basic standard output

Unit 6: Standard output.

This a general log of the model construction procedure, It contains tables displaying the input data, some performance (and possibly error) messages, and prints several tables of the output model. In most cases, these tables are self-explanatory.

The amount of output on Unit 6 is dependent upon input parameters. For instance, in the case where an LTE-grey model is generated (`LTEGR=.true`), there is a table containing the computed LTE-grey models. Another important portion of the output are tables containing various quantities produced if convection is taken into account.

The standard part of the output on Unit 6 (always present) is generated by the following subroutines: START, STATE (tables of input parameters); and OUTPRI (tables of resulting model parameters). For convenience, a part of this file is repeated on different output files. It concerns the performance and error messages (Unit 10), and emergent flux (Unit 81). This is useful either for a quick look if something went wrong (Unit 10), or for easy plotting (Unit 81). The basic quantities of the model itself appear on Unit 7.

Note: Unit 6, if accidentally or intentionally deleted, may to a large extent be re-created by a simple run of TLUSTY using unit 7 output as an input (unit 8), and with a modified unit 5 in which NITER=0, i.e. no iterations of complete linearization.

Unit 7: Condensed model atmosphere.

This is the basic output in a machine-oriented form, i.e. without any table headers, etc. It is created by subroutine OUTPUT. This file may serve as the model input to another run of TLUSTY as Unit 8, or to SYNSPEC and various interface and utility programs. Its structure is described in the previous Section.

Unit 9: Convergence log.

This is a very important output file, and the user is strongly encouraged to inspect it carefully after each run (there is also an IDL routine `RELC7` for plotting this file). The file is produced by subroutine PRCHAN. It contains, for each iteration of complete linearization, a table of relative changes in temperature, electron density, total particle density, the maximum relative change of all populations, the maximum relative change of all linearized mean intensities of radiation (i.e. those in the frequency points with IJALI = 0), the maximum relative change of all linearized quantities, and the indices of the level and the frequency point at which the respective maximum relative changes occur. All these quantities are printed as functions of depth. The relative change is defined as (new value - old value)/new value. The changes are printed in the order of decreasing depth index; this is because the linearized system is solved by the block-Gaussian elimination (forward elimination + backward substitution). To declare the computed model as well converged, the relative changes have to be gradually decreasing; in the last iteration they all have to drop below the prescribed value (10^{-3} being a reasonable value in most cases).

Unit 18 – Convergence log of the formal solution

Generated by subroutine RESOLV; the structure is similar as Unit 9, but it contains relative changes of populations only.

Unit 10: Performance and error log.

This file, created possibly by many different subroutines, contains messages about performance (log of accelerations, recalculation of the radiative equilibrium equation division optical depths, and all messages printed by the program when an error status occurs. These errors are either fatal (occurred when checking actual against maximum dimensions; calling various routines with inconsistent parameters; divergence of complete linearization); or warnings (slow convergence of subroutine ELCOR - a solution of the non-linear system of statistical equilibrium + charge conservation; negative opacities, etc.). All messages are more or less self-explanatory.

Unit 69: Timing.

As pointed out above, this file is produced only under Unix. In the distributed version of TLUSTY, the machine-dependent instructions are commented out, so that no file is created. In order to restore it the user has to delete the comment mark C at the first position of line number ... and .... The file is self-explanatory, and contains the time spent for the formal solution (with the subroutine RESOLV as a driver), and linearization SOLVE, together with the total time elapsed from the beginning of execution.

9.2 Auxiliary output

Unit 13 – Emergent flux.

Generated by subroutine OUTPRI in the final iteration. It prints the following quantities for all the frequency point, sorted by wavelength:

IJ – frequency index (original TLUSTY indexing)

FRQ – value of frequency (in s^{-1})

ALAM – wavelength (in Å)

FLUX – emergent flux, precisely the second moment of the specific intensity of radiation, H_ν, at the surface, in erg cm^{-2} $s^{-1}Hz^{-1}$

FH – the surface Eddington factor f_H, where $f_H = H_\nu(0)/J_\nu(0)$, $J_\nu(0)$ being the mean intensity of radiation at the surface

FLL – $\log H_\nu$

FLAM – $\log H_\lambda$; in erg $cm^{-2}s^{-1}Å^{-1}$

Unit 16 – Check of the statistical equilibrium.

Generated by subroutine CHCKSE in the final iteration. For each explicit level, it prints the total rate in and out, and their difference divided by the rate in, for each depth. The last column should contain much lower values than the previous two columns.

10 BENCHMARK TESTS

The basic means of obtaining program TLUSTY is to copy a package of files (the program plus benchmark tests) directly via anonymous ftp from `tlusty.gsfc.nasa.gov`.

The package consists of two subdirectories. One contains the source code for the program itself, the 'INCLUDE' files, and command procedures to run the program. The second contains all of the files for three bench tests, using old and new data formats.

The benchtest files include all of the input and output files required to calculate two model atmospheres from scratch.

First test model

The first selected model is a moderately complex model atmosphere with solar composition and the basic parameters:

effective temperature $T_{\text{eff}} = 25{,}000$ K
gravity $\log g = 4$

Hydrogen and helium are considered explicitly; C,N,O are considered implicitly, i.e. for the charge and particle conservation equations. We consider He I as a 14-level atom, while He II is assumed to be the highest ionization stage, with one level.

The calculation is done in two steps:

i) LTE model, starting with LTE-gray model,

ii) NLTE model, where one goes directly to NLTE model with lines, without an intermediate step of NLTE/continua only (NLTE/C), which was traditionally done in the past.

The files relevant to LTE model are denoted   `m25lt.*` (old format), and `n25lt.*` (new)
the files relevant to NLTE/L model   `m25nl.*` (old format), and `n25nl.*` (new)

The input files in both the "new" and the "old" formats are provided. Notice that the input is not exactly identical in these two cases. It is left to the user as an exercise to construct files which would provide the exactly identical input.

Second test model

This is an analogous model as above, but with including also 14 explicit levels of He II, and He III as 1-level ion (only in the "new" format). The input files are called `o25lt.*` and `o25nl.*`.

Other files

The directory also contains a script files `Testrun` and `T1` for running the whole set of benchmark tests under Unix.

Finally, we plan to provide a benchmark test for a line-blanketed model in a later release of this Guide.

APPENDIX – ATOMIC PARAMETERS

Photoionization cross-sections

The photoionization cross sections are evaluated as follows:

- for IBF $= 0$: $\sigma(\nu) = 2.815 \times 10^{-29} Z^4 \nu^{-3} n^{-5}$ (simplified hydrogenic)

- for IBF $= 1$: $\sigma(\nu) = 2.815 \times 10^{-29} Z^4 \nu^{-3} n^{-5} g_{\mathrm{II}}(n, \nu/Z^2)$ (exact hydrogenic)

- for IBF $= 2$: $\sigma(\nu) = \alpha[\beta x^s + (1 - \beta)x^{s+1}] \times 10^{-18}$ (Peach formula)

- for IBF $= 3$: $\sigma(\nu) = \alpha[\Gamma x^s + (\beta - 2\Gamma)x^{s+1} + (1 + \Gamma - \beta)x^{s+2}] \times 10^{-18}$ (modified Peach)

- for IBF $= 4$: $\sigma(\nu) = \exp[s + \alpha \log x + \beta \log^2 x]$ (Butler fit formula)

where $x = \nu_0/\nu$, s=SO, α=ALF, β=BET, and Γ=GAM. Parameter IBF is called IFANCY in subroutine START, SO, ALF, BET, GAM are input parameters. Further, n is the main quantum number, and Z the effective charge (=1 for neutrals, 2 for once ionized, etc.), and ν_0 the threshold frequency.

Collisional rates

Hydrogen:

- for ICOL $= 0$: standard expressions from Mihalas et al. (1975).

- for ICOL $= 1$: experimental fit formula for Lyα (Mihalas et al. 1975).

- for ICOL $= 2$: the Tschebyschev fit formula for Lyα after Crandall et al. (1974).

He I:

- for ICOL $= 0$: standard expressions from Mihalas et al. (1975).

- for ICOL $= 1, 2, 3$: Storey-Hummer fits to rates computed by Berrington and Kingston (1987). Data are given only for $n \leq 4$.

- for ICOL $= 1$: means that a given transition is a transition between non-averaged ls-states.

- for ICOL $= 2$: means that a given transition is a transition from non-averaged lower ls-state to an averaged upper state.

- for ICOL $= 3$: means that a given transition is a transition between two averaged states.

He II:

- for ICOL ≤ 0 : standard expressions from Mihalas et al. (1975).

Other elements:

Ionization:

- for ICOL $= 0$: $\Omega = 1.55 \times 10^{13} T^{-1/2} U_0^{-1} \exp(-U_0)\sigma_0$, $\sigma_0 \equiv$ OSC   (Seaton's formula)

- for ICOL $= 1$: $\Omega = c_0 T^{-3/2} U_0^{-2} \exp(-U_0)$, $c_0 \equiv$ OSC   (Allen formula)

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- for `ICOL` $= 2$: $\Omega = 5.465 \times 10^{-11} c_0 T^{1/2} \exp(-U_0)$, $c_0 \equiv$ `OSC`

- for `ICOL` $= 3$: $\Omega = 5.465 \times 10^{-11} c_0 T^{1/2} (1 + U_0) \exp(-U_0)$, $c_0 \equiv$ `OSC`

Excitation. In all cases, $f_{ij} \equiv$ `OSC`:

- for `ICOL` $= 0$: $\Omega = 19.7363 \, f_{ij} T^{-3/2} U_0^{-1} \exp(-U_0) max \left[\bar{g}, 0.276 \exp(U_0) E_1(U_0)\right]$; $\bar{g} = 0.25$

- for `ICOL` $= 1$: the same as above, but now $\bar{g}$ is an input parameter (`CPAR`) (van Regemorter formula)

- for `ICOL` $= 2$: $\Omega = 5.465 \times 10^{-11} f_{ij} c_0 T^{1/2} \exp(-U_0)$, $c_0 \equiv$ `CPAR`

- for `ICOL` $= 3$: $\Omega = 5.465 \times 10^{-11} f_{ij} c_0 T^{1/2} (1 + U_0) \exp(-U_0)$, $c_0 \equiv$ `CPAR`

- for `ICOL` $= 4$: $\Omega = 8.631 \times 10^{-6} g_i^{-1} T^{-1/2} \exp(-U_0) c_0$, $c_0 \equiv$ `CPAR` (Eissner-Seaton formula)

where $U_0 = (E_j - E_i)/(kT)$, E_i and E_j are the energies of the lower and upper level, g_i is the statistical weight, and f_{ij} the oscillator strength. Function E_1 is the first exponential integral function.

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