TLUSTY — A User's Guide

Version 202

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Contents

1 INTRODUCTION

The present set of computer programs is a package designed to accomplish a wide range of stellar spectroscopic diagnostics. 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. One of the most important features of the new version of the program is that it allows for a fully consistent, non-LTE metal line blanketing.

In the past, there was a separate variant called TLUSDISK, designed to calculate vertical structure of accretion disks. Starting at version 200, both programs are contained within a single, universal code TLUSTY. The user is able to make a choice between computing a model of a stellar atmosphere or an accretion disk based on input data. In the following text, we will usually refer to a "stellar atmosphere", but everything applies, unless specifically noted, for an accretion disk as well.

In its maximum configuration, the user may start from scratch and calculate a model atmosphere or a disk 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 second basic program is SYNSPEC, which is a program for calculating the spectrum emergent from a given model atmosphere. It has been originally designed to synthesize spectra from atmospheres calculated using TLUSTY, but may also be used with other model atmospheres as input (e.g. Kurucz's ATLAS models). The program is complemented by the program ROTINS which calculates the rotational and instrumental convolutions for the net spectrum produced by SYNSPEC.

Finally, there is a number of interface and utility programs. They provide a 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 to perform 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. The accompanying spectrum synthesis program SYNSPEC is described in a separate manual.

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 TLUSTY202. The previously distributed User's Guide described TLUSTY version 200.

The most important upgrades were already done in version 200, namely, a unification of TLUSTY and TLUSDISK, a possibility of including Compton scattering, a more consistent treatment of external irradiation, an introduction of level grouping, and, finally, a possibility of using the Opacity Sampling option to treat NLTE metal line blanketing. The differences between versions 200 and 202 are relatively subtle. We have changed the default for hydrogen collisional excitation rates and implemented most modern calculations by Przybilla & Butler (2004), allowed for charge transfer reactions, and allowed for collisional excitation by hydrogen atoms. Other changes concern mostly special cases, such as white dwarfs (various detailed hydrogen line profile treatments; equilibrium diffusion of helium, etc.), and very hot atmospheres.

2 GENERAL CHARACTERISTICS

2.1 Stellar Atmospheres

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; 2003). For a general review of computational strategies that allow to speed up the complete linearization refer to Hubeny & Lanz (2003).

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 formulas 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 numbers 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 a 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 the 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 evolved 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 of numerical techniques with respect to the original 1988 implementation.

- Unification of codes for stellar atmospheres and accretion disks

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

- Treatment of metal line blanketing, either by means of Opacity Distribution Functions (ODF – see Hubeny and Lanz 1995), or Opacity Sampling (OS). The ODF approach has been used in the past when the computer memory was insufficient (say below or around 512 MB of core memory); while in the present-day computer environment the Opacity Sampling is largely preferrable due to its higher accuracy and flexibility.

- Improved/added treatment of various physical features:

  - Convection (with several variants of the mixing length formalism)
  - External irradiation
  - Compton scattering (described in Hubeny et al. 2001)
  - Dielectronic recombination (described in Hubeny et al. 2001)
  - X-ray opacities, including the inner-shell (Auger) ionization

- 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).

2.2   Accretion Disks

The disk is assumed to be in steady state, geometrically thin and in Keplerian rotation. The vertical structure is solved for a set of axially symmetric concentric rings where a plane-parallel 1-D atmosphere calculation is performed.

Summarizing the basic assumptions:

- the disk is divided into a set of concentric rings, each behaving as an independent plane parallel radiating slab; no assumptions about optical thickness are made. One run of TLUSTY calculates the vertical structure of one ring;

- hydrostatic equilibrium in the vertical z-direction;

- energy balance is considered as a balance between net radiation loss (calculated exactly, without invoking neither optically thin, nor optically thick [diffusion] approximations), and dissipated mechanical energy;

- dissipated energy is proportional to viscosity, which is given through the traditional Shakura-Sunyaev (1973) α parameter; or through the Reynolds number;

- the effects of illumination of thedb disk by a central star are taken into account, using the formalism of Hubeny (1990b).

- In the case of accretion disks around black holes, we allow for general relativistic effects (we adopt here a formalism of Riffert and Herold 1995). The structural equations are described in detail in Hubeny and Hubeny (1998).

2.3 Approximate models

For many purposes, one does not need detailed self-consistent models of the disk vertical structure as described above, but rather some approximate models. One possibility is the so-called LTE-grey model (which is used as a starting model for subsequent iterative calculations of the self-consistent vertical structure). The model is described in detail in Hubeny (1990a). To calculate such a model, the user has to code `NITER=0`, i.e. no iterations of the complete linearization (or the hybrid CL/ALI method - see below) are performed.

An even simpler model is the isothermal slab model. The model is similar to the grey model, but the temperature is assumed constant with height, having a prescribed input value. An isothermal model may be calculated either in the LTE-grey approximation, or by solving all other structural equations (assuming LTE or NLTE). In the later case, the user has to code `INRE=0` (see below), which has the effect of keeping the temperature fixed in the linearization process.

2.4 Word of Caution

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 the program as a "black box". It would be highly appreciated if any errors detected by the user, and any comments or suggestions for improvements, are communicated to I. Hubeny (`hubeny@aegis.as.arizona.edu`) or T. Lanz (`lanz@astro.umd.edu`).

3 COMPILING AND LINKING

3.1 Compilation

The program is distributed as several files. The largest is `TLUSTYnnn` where `nnn` represents the current version number. In the following text, we take 202 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 `tlusty202.f` file, and, under UNIX, their names *must* be in capital letters, e.g. `BASICS.FOR`. We stress that the INCLUDE files generally

evolve together with TLUSTY (more parameters are being added), so that the user is advised to copy these files along any new version of TLUSTY.

The compilation and linking is done as follows:
• under UNIX

```
f77 [-O4] [-static] [-Nl100] tlusty202.f
```

where the option `"-Nl100"` is sometimes needed under older variants of the SUN operation system (increases the number of continuation lines to 100); the option `"-static"`, which is needed for some variants of UNIX, indicating a static allocation of memory. It is now a 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 LINUX

```
g77 -fno-automatic [-O3] tlusty202.f
```

where the option `"-fno-automatic"`, which is the analog of the `"-static"` option, is necessary, since it is not the default in most implementations of g77.

One may also use the commercial Portland Group compiler, pgf77, which provides better optimization (the code is typically 20-30% faster);

```
pgf77 -Wl -Bstatic [-fastsse]  tlusty202.f
```

3.2 Reducing the size of the executable file

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
MDEPTH	maximum number of depth points
MFREQ	maximum number of frequencies
MFREQC	maximum number of frequencies in continua
MFREX	maximum number of linearized frequencies
MFREQL	maximum number of frequencies per line
MMU	maximum number of angle points
MMUC	maximum number of angle points (in case of Compton scattering)
MTRANS	maximum number of all transitions which are somehow taken into account
MBF	maximum number of bound-free transitions
MCROSS	maximum number of photoionization cross-sections + related quantities
MFIT	maximum number of fit points for input of bound-free cross-sections
MMCDW	maximum number of levels with pseudocontinuum
MMER	maximum number of "merged" levels
MZZ	maximum charge of an ion treated with occupation probabilities
MITJ	maximum number of overlapping lines

MVOIGT maximum number of lines with Voigt profiles
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 above parameters are universal. There are also other parameters which specify dimensions of arrays which are being used only under special circumstances (including Compton scattering; tri-diagonal approximate operatore, etc.), which in set to 1 for the bulk of applications. These are the following:

MDEPTC set to MDEPTH in case of Compton scat, otherwise =1
MFREQ1 set to MFREQ in case of Compton scattering or DFE transfer solver; otherwise =1
MLEVE3 set to MLEVEL in case of tridiagonal operator; otherwise =1
MLVEX3 set to MLVEXP in case of tridiagonal operator; otherwise =1
MTRAN3 set to MTRANS in case of tridiagonal operator; otherwise =1

In addition, there are several parameters in INCLUDE file `ODFPAR.FOR` that specify array dimensions for a treatment of metal line blanketing. They are the following:

MFODF maximum number of frequency points per ODF
MDODF maximum number of depth points for storing the ODF's
MHOD maximum number of merged-levels ODF's
MKULEV maximum number of internal energy levels for an ion treated by means of opacity
    sampling; if opacity sampling is not used, should be set to 2
MLINE maximum number of internal lines for an ion treated by means of opacity
    sampling; if opacity sampling is not used, should be set to 2
MCFE maximum total number of internal lines for all ions treated by means of opacity
    sampling; if opacity sampling is not used, should be set to 2

Finally, there is one parameters in INCLUDE file `MODELQ.FOR` that specifies the total number of internal frequency points for treating metal lines in the Opacity Sampling approach:

MFREQP maximum number of internal frequency points for Opacity Sampling

This value is set by default to MFREQ, but in some cases needs to be larger.

The program checks whether the current values are less than the corresponding maximum dimension, and stops if there is a conflict. The program then issues a brief message (on standard output), showing the corresponding current and maximum values. The program should then be recompiled with the corresponding parameter appropriately modified in file `BASICS.FOR` or `ODFPAR.FOR`.

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.

A reduction of the size of the executable file is accomplished by reducing some of the above parameters specifying array dimensions (in "include" files `BASICS.FOR` and `ODFPAR.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 $MSMX \times MSMX \times ND \times 3$ words), with a relatively insignificant increase of computer time (of the order of $10 - 20\%$). We stress again that when one computes a model without the Opacity Sampling treatment of line blanketing due to the iron-peak species, the parameters `MKULEV, MLINE`, and `MCFE` in the file `ODFPAR.FOR` should be set to 2 which leads to a significant reduction of the size of the executable file.

4 GENERAL SCHEME OF THE INPUT

4.1 Overview

Version 200 of TLUSTY ceased to support the so–called "old" format of input which was supported before; the only allowed format is the "new" one.

CAUTION: Previous Unit 1 input file (fort.1), which had the meaning of a switch indicating whether the old or new format of input is being used, has now the meaning of a switch determining whether an atmosphere or an accretion disk model is computed.

The basic feature of the 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 the optional (or sometimes called "non-standard") parameters are set up. Optional parameters are defined as those for which the program assigns default values, which are optimum for most applications, but could be changed as required for a particular special application, or to choose among several alternative numerical schemes, or to cope with convergence problems.

- Unit 1 — The basic control file, containing just one single number, specifying whether one calculates a stellar atmosphere or accretion disk model. If this number is 0, or if the file is missing altogether, the programs assumes that a stellar atmosphere model is to be computed. Otherwise, a disk vertical structure is computed.

- Unit 5 — Main control data – a short file with only the most important parameters, and filenames of other files. The structure of the file and the meaning of the individual input parameters is explained in Sect. 5.

- Files containing atomic data for the individual ions. These files are discussed in Sect. 8. As discussed in that Section, a collection of such files is available on the TLUSTY website at `http://nova.astro.umd.edu`.

- File containing non-default values of the optional parameters (if needed). There are altogether more that 160 possible optional parameters; they are discussed in detail in Sect. 6

- Unit 8 — A starting model atmosphere (if needed) - see Sect. 9.

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.

4.2 What needs to be specified?

There are two types of input parameters; the true *physical quantities* (such as the effective tempera-
ture, T_{eff}), and *control parameters* – typically flags that switch on/off various numerical procedures,
control the choice of adopted numerical scheme, etc.

We stress that a NLTE stellar atmosphere code is not a black box. The setup of the model
depends to a large extent of user's judgment (e.g., determining a degree of sophistication of the
model). The user has to understand the meaning of a number of input parameters. The philosophy
behind introducing several input files is an attempt to help a user in such a way that only truly
important parameters have to be set up in the standard input file, while other, less important
parameters, assume their default values unless the user specifically requires to change them. This
is done through the optional parameters file.

We list the essential categories of the input parameters below.

- Basic model parameters.
  These are T_{eff} and $\log g$ for stellar atmospheres, and analogous parameters for accretion disks.
  These are of course mandatory, and are communicated to TLUSTY through the standard
  input – see Sect. 5.1.

- Setting LTE or NLTE.
  This is done in standard input, see Sect. 5.1.

- Chemical composition and the choice of explicit species.
  The *explicit* atom is defined as such for which a selected set of energy levels of a selected set of
  its ionization states are considered explicitly, i.e., their populations are determined by solving
  statistical equilibrium. These species are the only ones that are allowed to contribute to
  the total opacity, so their choice is important because when neglecting an important opacity
  source the quality of the resulting model will suffer. An *implicit* atom is not allowed to
  contribute to the 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.
  The choice of explicit and implicit atoms, together with their abundances, is given at the
  standard input – see Sect. 5.3.

- Choice of explicit ions.
  Again, the choice has to be made judiciously; otherwise the quality of the model decreases.
  The choice is also given in the standard input – see Sect. 5.4.

- Atomic data for explicit ions.
  This is an important, and sometimes decisive, ingredient of good NLTE models. In early
  versions of TLUSTY, the atomic data were communicated in the standard input file. This
  became too cumbersome when the model atoms became very extended, so the so-called "new"
  system of input (starting from version 200, now the only supported system) contains in the
  standard input file only the filenames of the individual atomic data for each explicit ion;
  the atomic/ionic data files are separate. This enables us to store those files and distribute
  them together with the program. This is actually done on the TLUSTY website, where a
  collection of such files, in varying degree of sophistication and complexity, is presented. The
  user can thus use those files without being required to construct them. The atomic data files
  also contain a mixture of physical parameters (such as the level energies, oscillator strengths,
  etc.), and also control parameters for switching particular options. Therefore, in some cases

one may need to modify the atomic data file to set up a different option if required (for instance, setting a different choice of level grouping - see Sect. 7.1).

- Auxiliary physical parameters.
  Here we have for instance convective parameters, microturbulent velocity, possible external irradiation intensity, etc. As explained in the next Sections, the user has a choice of including or not including these physical mechanisms at all, and if so, to set up corresponding numerical values. These parameters are communicated through the optional flag file, discussed in detail in Sect. 6.

- Basic discretization parameters.
  This category contains the number of depth, frequency, and angle points used when discretizing the corresponding structural equations. The number of depth and angle points are set up by corresponding optional parameters. The actual values of the individual column masses (which is the standard means to express depth in the atmosphere) are either given in the input model, or are constructed in the starting LTE-grey model atmosphere. The corresponding parameters are also set up in the optional parameters - see Sect. 6.3. If none are specified, the default values are adopted. The total number of frequency points is set up by TLUSTY, and depends on the actual selection of lines and continua that are treated explicitly. The user can influence some aspects of the selection via the standard input – see Sect. 5.2, and through several optional parameters – see Sect. 6.2 and 6.11.

- Numerical options
  There is a large number of flags for controlling many numerical aspects, usually communicated as optional parameters – see Sect. 6 and 7. As mentioned above, the atomic data files also contain some flags of this category. If the model computation proceeds well without any special optional flags file, that is if the default values of optional parameters provide a satisfactory numerical strategy, the user does not have to set up this file. However, in a number of cases one needs to set up some optional parameters, so one is recommended to obtain at least a rudimentary knowledge from Sect. 7; more dedicated users are encouraged to study also Section 6 in detail.

5   STANDARD INPUT

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

5.1   First block – Basic Parameters

This block contains only three lines of input.

- **1st line:**

This is the only input record that differs for atmospheres and disks; all the other input values have the same meaning for both basic options.
•• For stellar atmospheres:

TEFF – effective temperature [K]

GRAV – $\log g$ [cm s^{-2}]

•• For accretion disks:

XMSTAR – mass of the central object. There are still three possibilities:

- XMSTAR > 0 – in this case the central object is supposed to be a star; computation of the structure is done in the classical approximation. The mass can be expressed either in grams, or in solar masses.
- XMSTAR < 0 – in this case the central object is a black hole; computation of the structure is done using general relativistic corrections. The mass of the black hole is then abs(XMSTAR); again, it is expressed either in grams or in solar units.
- XMSTAR = 0 – in this case the meaning of the subsequent four quantities of the input is different; instead of using basic parameters M_*, $\dot{M}$, R_*, and R/R_* or R/R_g), one uses specific parameters for an annulus without explicit reference to the central object, namely T_{eff}, Q, and m_0.

XMDOT – mass accretion rate. Can be expressed in g/s, or in $M_\odot/\text{yr}$

RSTAR – again, two different meanings depending whether one considers a classical or general relativistic central object.
• In the classical case, RSTAR is the radius of the central star (in cm or in $R_\odot$);
• in the case of a black hole accretion, RSTAR has the meaning of the spin (angular momentum) of the black hole, expressed in geometrized units (i.e. =0 for a Schwarzschild black hole; =0.998 for a maximum rotating Kerr black hole)

RELDST – relative distance of a given annulus with respect to the stellar radius (classical case) or gravitational radius (for the black hole case). Gravitational radius is defined by $R_g = GM/c^2$. Caution: the Schwarzschild radius, which is being used by some authors as a reference radius, is given by $R_S = 2R_g$

In the alternative case, when XMSTAR = 0, the subsequent three numbers in the first line of input have the following meaning:

TEFF – effective temperature [K]

QGRAV – the proportionality coefficient, Q, to evaluate the z-dependent gravity acceleration, $g = Qz$. In the classical case, $Q = \Omega_K^2$, where Ω_K is the Keplerian velocity, $\Omega_K = (GM/R^3)^{1/2}$

DMTOT – column mass at the midplane [g]

• **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 optional parameters.
    = '' (null string) – all optional parameters are taken with their default values – see the next
    section.

5.2   Second block – Frequencies

This block usually contains 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 optional
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. The details of setup are
    governed by several optional parameters (FRCMAX, FRCMIN, CFRMAX, NFTAIL, and
    DFTAIL – see Sect.6.2). In the default case, the program sets two frequencies near disconti-
    nuities corresponding to the bound-free transitions form all explicit levels, plus approximately
    NFREAD frequencies in between, plus a number of points in the high- and low-frequency
    tails of the spectrum. The endpoints of the high- and low-frequency tails are specified by
    the optional parameters FRCMAX and FRCMIN, respectively; the number of points in the
    high-frequency tail are specified by the optional parameters NFTAIL and DFTAIL. (i.e. they
    may be changed by a corresponding specification in the input file FINSTD).
    In the case of NFTAIL < 0, there are exactly NFREAD frequency points, set up logarithmi-
    cally equidistant between FRCMIN and FRCMAX.
    < 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 for describing the continuum (if one considers lines, the
line frequencies are set up automatically), 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 § 8.2.

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

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) 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.

  ii) 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.

  iii) 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 (the points immediately shortward of the edges) to be linearized. In some cases, it is not necessary to select any points to be linearized.

5.3   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.). At present, TLUSTY treats only elements with atomic number 1 – 30, i.e., H – Zn. It is planned to allow for all chemical species in the future.

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

  0. not considered at all.

  1. 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.

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

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 0);
    = 1 – if the element is non-explicit (option 1);
    = 2 – if the element is explicit (option 2).

ABN – a specification of abundance of the given species:
    = 0 – the solar abundance is assumed (Grevesse & Sauval 1998);
    < 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 $N(\text{elem})/N(\text{ref})$, i.e. relative by number to the reference species. The reference atom is H by default, but the reference species can be changed by mean of the optional parameter IATREF (see Sect. 6.6)
    > 10^6 – non-homogeneous (depth-dependent) abundance is assumed. In this case, the following ND 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.

5.4   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 has to 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 block.

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) or Opacity Sampling (OS) 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 or OS 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.

5.5 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). The absolute value of IUPSUM specifies the main quantum number of the highest hydrogenic level considered. 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 files. If they are zero, the program assigns the unit numbers automatically.

FIODF1, FIODF2 – filenames for super-line data:

– in the case of ODF treatment of lines, the filenames of the corresponding ODF input;

– in the case of OS, the first file is Kurucz level data file (e.g., `gf2601.gam`, for Fe II), and the second file is the line data file (`gf2601.lin`).

FIBFCS – the name of the file containing the photoionization cross-sections for the individual superlevels. The parameters IFANCY (see Sect. 8.2) has 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 and OS input files is given in Sect. 6.11.

5.6 An example

A simple LTE model atmosphere with $T_{\text{eff}} = 35{,}000$ K, $\log g = 4$, composed of H and He only, may be constructed by TLUSTY202 by coding the standard input as follows:

```
35000. 4.0          ! TEFF, GRAV
T  T                ! LTE,  LTGRAY
''                  ! no change of general optional 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 $h\nu_{\max}/kT_{\text{eff}} = 38$ – 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.

5.7 Another example: NLTE line-blanketed O star model atmosphere

A complex example is provided for a NLTE line-blanketed O star model atmosphere, with $T_{\text{eff}} = 35{,}000$ K, $\log g = 4$, with a metallicity a fifth solar. This example corresponds to the data used for calculating the OSTAR2002 grid (Lanz & Hubeny 2003).

```
35000. 4.0
 F  F                 ! LTE,  LTGRAY
 'nst'                ! name of file containing non-standard flags
```

```
*
* frequencies
*
 2000
*
* data for atoms
*
 30                      ! NATOMS
* mode abn modpf
    2   0.        0        ! H
    2   0.        0         ! He
    0   0.        0
    0   0.        0
    0   0.        0
    2  -0.2       0  ! C
    2  -0.2       0  ! N
    2  -0.2       0  ! O
    1  -0.2       0
    2  -0.2       0  ! Ne
    1  -0.2       0
    1  -0.2       0
    1  -0.2       0
    2  -0.2       0  ! Si
    2  -0.2       0  ! P
    2  -0.2       0  ! S
    1  -0.2       0
    1  -0.2       0
    1  -0.2       0
    1  -0.2       0
    1  -0.2       0
    1  -0.2       0
    1  -0.2       0
    1  -0.2       0
    1  -0.2       0
    2  -0.2       0  ! Fe
    1  -0.2       0
    2  -0.2       0  ! Ni
    1  -0.2       0
    1  -0.2       0
*
* data for ions
*
*iat   iz   nlevs  ilast ilvlin  nonstd typion  filei
*
   1    0     9       0      0       0     ' H 1' 'data/h1.dat'
   1    1     1       1      0       0     ' H 2' ' '
   2    0    24       0      0       0     'He 1' 'data/he1g.dat'
   2    1    20       0      0       0     'He 2' 'data/he2g.dat'
```

```
 2    2     1      1      0      0    'He 3' ' '
 6    1    22      0      0      0    ' C 2' 'data/c2g.dat'
 6    2    23      0      0      0    ' C 3' 'data/c3g.dat'
 6    3    25      0      0      0    ' C 4' 'data/c4g.dat'
 6    4     1      1      0      0    ' C 5' ' '
 7    1    26      0      0      0    ' N 2' 'data/n2g.dat'
 7    2    32      0      0      0    ' N 3' 'data/n3g.dat'
 7    3    23      0      0      0    ' N 4' 'data/n4g.dat'
 7    4    16      0      0      0    ' N 5' 'data/n5g.dat'
 7    5     1      1      0      0    ' N 6' ' '
 8    1    29      0      0      0    ' O 2' 'data/o2g.dat'
 8    2    29      0      0      0    ' O 3' 'data/o3g.dat'
 8    3    39      0      0      0    ' O 4' 'data/o4g.dat'
 8    4    40      0      0      0    ' O 5' 'data/o5g.dat'
 8    5    20      0      0      0    ' O 6' 'data/o6g.dat'
 8    6     1      1      0      0    ' O 7' ' '
10    1    15      0      0      0    'Ne 2' 'data/ne2g.dat'
10    2    14      0      0      0    'Ne 3' 'data/ne3g.dat'
10    3    12      0      0      0    'Ne 4' 'data/ne4g.dat'
10    4     1      1      0      0    'Ne 5' ' '
14    2    30      0      0      0    'Si 3' 'data/si3g.dat'
14    3    23      0      0      0    'Si 4' 'data/si4g.dat'
14    4     1      1      0      0    'Si 5' ' '
15    3    14      0      0      0    'P  4' 'data/p4g.dat'
15    4    17      0      0      0    'P  5' 'data/p5g.dat'
15    5     1      1      0      0    'P  6' ' '
16    2    20      0      0      0    ' S 3' 'data/s3g.dat'
16    3    15      0      0      0    ' S 4' 'data/s4g.dat'
16    4    12      0      0      0    ' S 5' 'data/s5g.dat'
16    5    16      0      0      0    ' S 6' 'data/s6g.dat'
16    6     1      1      0      0    ' S 7' ' '
26    2    50      0      0     -1    'Fe 3' 'data/fe3v.dat'
 0    0                              'data/gf2602.gam'
                                     'data/gf2602.lin'
                                     'data/fe3p_22+7lev.rap'
26    3    43      0      0     -1    'Fe 4' 'data/fe4v.dat'
 0    0                              'data/gf2603.gam'
                                     'data/gf2603.lin'
                                     'data/fe4p_21+11lev.rap'
26    4    42      0      0     -1    'Fe 5' 'data/fe5v.dat'
 0    0                              'data/gf2604.gam'
                                     'data/gf2604.lin'
                                     'data/fe5p_19+11lev.rap'
26    5    32      0      0     -1    'Fe 6' 'data/fe6v.dat'
 0    0                              'data/gf2605.gam'
                                     'data/gf2605.lin'
                                     'data/fe6b.rap'
26    6     1      1      0      0    'Fe 7' ' '
```

```
   28     2     36      0       0       -1      'Ni 3' 'data/ni3v.dat'
    0     0                                            'data/gf2802.gam'
                                                       'data/gf2802.lin'
                                                       'data/ni3.72'
   28     3     38      0       0       -1      'Ni 4' 'data/ni4v.dat'
    0     0                                            'data/gf2803.gam'
                                                       'data/gf2803.lin'
                                                       'data/ni4.73'
   28     4     48      0       0       -1      'Ni 5' 'data/ni5v.dat'
    0     0                                            'data/gf2804.gam'
                                                       'data/gf2804.lin'
                                                       'data/ni5.74'
   28     5     42      0       0       -1      'Ni 6' 'data/ni6v.dat'
    0     0                                            'data/gf2805.gam'
                                                       'data/gf2805.lin'
                                                       'data/ni6.75'
   28     6      1      1       0        0      'Ni 7' ' '
    0     0      0     -1       0        0      '     ' ' ' '
*
* end
```

The optional parameters (see Sect.6) used are

```
NLAMBD=3,ND=50,VTB=10.,ISPODF=1,DDNU=0.75,CNU1=6.
```

The model atmosphere includes 11 explicit atoms, 45 explicit ions, and 907 explicit NLTE (super)levels. Opacity Sampling is used (ISPODF=1), with a typical step of 0.75 fiducial Doppler width for iron. The whole spectrum is represented by 184,136 frequencies. The radiation field mean intensity is linearized at 17 frequencies.

6   OPTIONAL PARAMETERS

There are about 160 different optional parameters. We repeat that an optional 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 optional parameters are actual physical parameters, like the convective mixing length, or the microturbulent velocity, which are zero for most applications. However, the majority of optional 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 optional 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 optional parameters into the following 14 categories.

1. Auxiliary physical parameters

2. Automatic setup of frequency points

3. Specification of the LTE-gray model

4. Flags for modifying the starting model atmosphere

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 for a treatment of line blanketing

12. Non-standard atomic transition rates; hydrogen line profiles

13. Parameters specifying the global acceleration schemes

14. Miscellaneous auxiliary parameters

15. Parameters determining an amount of additional output

The file, whose name is specified by the standard parameter FINSTD (see the previous Section), contains a list of the optional 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.

Hint: Since parameters to be changed has to be specified by capital letters. changing one letter to a lower case may be used as a way of "commenting out" a given parameter, which can than easily be reinstated later. For instance, coding

```
ITEK=8
```

has the effect of starting the Kantorovich acceleration (see Sect.6.13) at 8th iteration; while setting
```
ITE=8   or   itek=8   or   iTEK=8
```
has no effect, and ITEK will assume its default value (ITEK=4).

In the rest of this Section, we will describe all the individual optional parameters in detail, including their default values. Finally, we list some of the most important optional parameters, which are most likely to be changed when one encounters convergence difficulties.

6.1 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.

MLTYPE – switch for the type of the mixing length prescription:
$= 0$ or 1 – normal mixing length (type 1);
$= 2$ – the so-called ML2 prescription (Fontaine et al 1981; Bergeron et al. 1992)
DEFAULT: MLTYPE=0.

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.

IPTURB – switch for setting the effects of microturbulent velocity:
$= 0$ – the turbulent velocity is considered only for modifying the Doppler widths, but not for turbulent pressure (which is set to zero);
$= 1$ – the turbulent velocity is considered both for Doppler widths as well as for determining the turbulent pressure via $P_{\text{turb}} = (1/2)\rho v_{\text{turb}}^2$
DEFAULT: IPTURB=1.

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 $I_\nu^{\text{irrad}} = W B_\nu(T^*)$, 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: TRAD =0.

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

• Parameters specific to white dwarf models. They account for equilibrium diffusion of helium and thus construct enable to compute models with helium stratification, by specifying the total mass of the layer of hydrogen that floats on a helium layer. The formalism is taken from Vennes et al. (1988).

HCMASS – if set to a non-zero value, the total mass of the hydrogen layer (in g or in $M_\odot$) for stratified H-He models with equilibrium helium diffusion.
$= 0$ – no helium stratification
DEFAULT: HCMASS=0.

RADSTR – stellar radius (in units of the solar radius) of the star (for stratified models with equilibrium helium diffusion)
DEFAULT: RADSTR=0.

- Parameters specific to disk models:

ALPHAV – viscosity parameter α. If > 1, then ALPHAV has the meaning of the Reynolds number. DEFAULT: ALPHAV=0.1

IVISC – a mode of treating depth-dependent viscosity:
≥ 0 – the depth-averaged viscosity is determined through the "averaged" α, given by the parameters ALPHAV; while the depth dependence of kinematic viscosity is treated as a two-step power law as described by Hubeny & Hubeny 1998. In this case, one needs to specify four more parameters: two power-law exponents ζ_0 and ζ_1; the division point DMVISC; and the fraction of energy dissipated in the inner layer, FRACTV – see below.
$= 2$ – the local viscous stress is given by $t_{\phi r} = \alpha P_{\text{gas}}$; i.e. α determines the *local* viscosity. Additional details are given in the Appendix 2.
DEFAULT: IVISC=0

ZETA0 – the viscosity parameter ζ_0
DEFAULT: ZETA0=0 (viscosity constant in the inner layers).

ZETA1 – the viscosity parameter ζ_1
DEFAULT: ZETA1=0 (viscosity constant in the outer layers).

FRACTV – the viscosity parameter f; i.e. the fraction of energy dissipated in inner layers (with the power-law exponent ζ_0);
if < 0 – the kinematic viscosity is assumed to be a continuous function of depth, and FRACTV is computed through the division mass DMVISC;
DEFAULT: FRACTV=-1

DMVISC – the division mass m_0 in the viscosity prescription. (expressed as m_0/m_{tot}, where m_{tot} is the column mass at the disk midplane).
DEFAULT: DMVISC=0.01 (i.e. 1% of the total column mass is considered as "outer layers").

IZSCAL – switch determining whether the basic depth scale is given by the column mass, m, or a geometrical distance, z.
$= 0$ – the basic scale is the m-scale. In this case, the total column mass at the midplane is computed in the LTE-grey model (or is read from the input model), and is held fixed.
$= 1$ – the basic scale is the z-scale
DEFAULT: IZSCAL=0

6.2   Automatic setup of frequency points

FRCMAX – the maximum frequency.
$= 0$ – maximum frequency is set up such as
a) for atmospheres: $\nu_{\max} = 8 \times 10^{11} T_{\text{eff}}$; i.e. $h\nu_{\max}/kT_{\text{eff}} \approx 38$;
b) for accretion disks: $h\nu_{\max}/kT_{\text{mid}} = 17$, where T_{mid} is the local temperature at the midplane (evaluated approximately through the effective temperature and the total column density Σ as $T_{\text{mid}} = 2.83 \times 10^{11} T_{\text{eff}} (0.2\,\Sigma)^{1/4}$ $h\nu_{\max}/(kT_{\text{eff}}) = 38$ (see Hubeny et al. 2001).
> 0 – the value of maximum frequency.
If another optional parameter CFRMAX is set to a value larger than 1, the maximum frequency is then set to maximum of the above and CFRMAX times the frequency of the explicit photoionization edge with the highest-frequency.
DEFAULT: FRCMAX=0.

CFRMAX – auxiliary parameter for setting the maximum frequency – see above
  DEFAULT: CFRMAX=2 for atmospheres; =0 for disks

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

FRLMAX – the maximum frequency in the line transitions.
  = 0 – the maximum frequency in the line transitions is set to FRCMAX.
  > 0 – the value of maximum frequency in the line transitions
  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}.
  > 0 – the value of minimum frequency in the line transitions
  DEFAULT: FRLMIN=10^{13}

NFTAIL – one of parameters that determine the automatic setting of frequency points.
  > 0 – it has the meaning of the number of frequency points between the highest-frequency continuum edge and the maximum frequency given by parameter `FRCMAX` – see above. In this case, the frequencies are set up in such a way that each continuum edge is represented through two frequency points immediately above and below the edge, plus the high- and low-frequency tails, plus some frequencies between edges (see also description of parameter `NFREQ` of the standard input).
  The integration is done by the Simpson formula, so that NFTAIL must be an odd number. Specifically, the integration 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 the photoionization edge is DFTAIL times the total interval. This allows one to consider denser grid of frequency points just blueward of the highest-frequency discontinuity, which yields more accurate evaluation of the photoionization rate of the corresponding transition.
  < 0 – the frequencies are set as equidistant in $\log \nu$ between the minimum and maximum frequency. The total number of frequency points is now exactly `NFREQ`. This option is very useful for hot disks, for which the previous option would generate an unnecessarily large number of frequencies around completely unimportant edges.
  DEFAULT: NFTAIL=21

DFTAIL – see above.
  DEFAULT: DFTAIL=0.25

6.3   LTE-grey model input

For stellar atmospheres:

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 (this has only a pedagogical significance).
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 and 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: IH2=0

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

For accretion disks:

DM1 – the column mass in the first depth point.
DEFAULT: DM1=1.d-3

ABPLA0 – the initial estimate of the Planck mean opacity (per gram) at the first depth point.
DEFAULT: ABPLA0=0.3

ABPMIN – minimum value of the Planck mean opacity.
DEFAULT: ABPMIN=1.d-5

ITGMAX – the number of internal iterations in computing the LTE-grey model.
DEFAULT: ITGMAX=10

NNEWD – indicator of changing the depth grid in the LTE-grey model.
= 0 – the grid is set up once and for all and is not changed;
> – the grid is updated NNEWD times.
DEFAULT: NNEWD=0

TDISK – if set to be non-zero and positive, it has the meaning of the temperature of the disk, assumed constant with height (it is that a means to compute the hydrostatic structure of an isothermal disk)
DEFAULT: TDISK=0 (i.e., the temperature structure is determined by solving the energy balance equation)

Other parameters, ABROS0, NDGREY, IDGREY, IHM, IH2, and IH2P, have the same meaning as in the atmospheric case.

6.4   Flags for modifying 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 § 9.
= 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 § 9.
= 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 – a "simple" change of the level structure – levels are only added, and only for new species;
< 0 – change of the structure; a detailed additional input for each level of the present run is required.
DEFAULT: ICHANG=0

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

NMU – number of angle points for the formal solution of the transfer equation; using the Gaussian quadrature in angles
DEFAULT: NMU=3

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=1

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^* (this option was not properly tested in version 202; does not work properly for some setups).
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).
$= -1$ – al points are in the linearized mode, regardless of other input (i.e., the original complete linearization method). 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 ≥ 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 ≥ 3.

DEFAULT: NTRALI=3

6.6 Flags for selecting a treatment of the statistical equilibrium equations

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). IATREF refer to the *index* of the atomic species in the numbering of explicit species. Therefore, for instance, if H is not considered explicitly at all (mode 0 or 1) and He is explicit, then the index IAT for He is set to 1, and the IATREF should be set to 1 (which is a default anyway).

$= 0$ – 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

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 for NLTE models; IFLEV=1 for LTE models

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 (this option is not supported in version 202, and thus should not be used).
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

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

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)

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 $n^{\mathrm{new}} = n^{\mathrm{old}} + \Delta n$) 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

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-30

POPZR2 – a secondary parameter for setting up a level zeroing.
DEFAULT: POPZER=1.e-30

NITZER – iteration number till which the population can be zeroed or un-zeroed. After NITZER-th iteration, any new zeroing is switched off, so the populations that were already zeroed at this iteration stay zeroed till the end of the run DEFAULT: NITZER=3

RADZER – an analogous parameter for zeroing the mean intensity. This option avoids numerical problems connected with extremely small intensity at the highest frequencies, in particular for accretion disks. When mean intensity decreases below RADZER times the maximum relative intensity, it is set to zero.
DEFAULT: RADZER=1.e-20

6.7   Parameters for the global iteration loop control

ND – number of depth points
DEFAULT: ND=70

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

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=0.01

NLAMT – the reset number of lambda iterations – see above.
DEFAULT: NLAMT=1

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), This option is kept for historical reasons only;
> 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

NELSC – a mode of treating the electron scattering by the Feautrier scheme (it has no meaning for the DFE scheme, ISPLIN $\geq$ 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 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. This option is kept for pedagogical and historical reasons only.
> 0 – derivatives are calculated.
DEFAULT: IBPOPE=1

DPSILG – during linearization, the relative changes of all state parameters are artificially limited not to exceed certain values. DPSILG sets up a general limit for all quantities, in a sense that $\delta(\psi_i)/\psi_i = \max[1/\text{DPSILG} - 1, \delta(\psi_i)/\psi_i]$; $\delta(\psi_i)/\psi_i = \min[\text{DPSILG} - 1, \delta(\psi_i)/\psi_i]$;
DEFAULT: DPSILG=10. (i.e. all the relative changes are truncated to have values between -0.9 and 9.)

DPSILT – analogous, but limits specifically the relative changes in temperature. If DPSILT < DPSILG, DPSILT overwrites DPSLIG.
DEFAULT: DPSILT=1.25

DPSILN – analogous, but for relative changes of electron density.
DEFAULT: DPSILN=10.

DPSILD – analogous, but for the logarithmic gradient Δ (effective only if convection is switched on, ICONV $\neq$ 0.
DEFAULT: DPSILD=1.25

6.8   Parameters for setting up the linearization matrices

The following parameters INHE, INRE, INPC, INSE, INMP, INDL, INZD, 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 or disks)

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

INZD – a position of z – vertical distance from the midplane. Used for disk models only. DEFAULT: INZD=0 for atmospheres; INZD=4 for disks.

IFIXMO – a shortcut for setting all parameters INHE, INRE, INPC, and (for disks) INZD, to zero. It happens if IFIXMO is set to a non-zero value.
DEFAULT: IFIXMO=0

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

6.9 Additional opacities

IOPADD – a switch for calculating additional opacities:
= 0 – no additional opacities are calculated, regardless of what the following parameters say. In other words, to allow for instance for the Rayleigh scattering opacity, one has to set not only IRSCT=1 (see below), but also IOPADD=1. If one sets IRSCT=1 and IOPADD=0, the Rayleigh scattering is still neglected.

> 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

6.10 Parameters defining a numerical treatment of convection

ICONV – a flag to switch on the convection:
$= 0$ – convection is neglected. However, if the optional parameter HMIX0 is set to a positive value, ICONV is reset to ICONV=1.
> 0 – convection is considered, and is linearized. There are several numerical options, but they are at the moment experimental. The user is recommended to use value ICONV=1 (which is set automatically if the parameter HMIX0 is set).
Note: if ICONV is set to ICONV >0, but HMIX0=0, then all convective routines are called, but the convective flux will always be zero, so effectively no convection is allowed for.
< 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 $T^{\text{new}} = T^{\text{old}} + \Delta(T)$ (as it is done without convection);

= 1 – new temperature is calculated through the logarithmic gradient DELTA in the convection zone (DELTA $\equiv \Delta = d \ln T / d \ln P$);
= 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

ICONRE – if set to a positive value, a routine CONREF is called that recalculates temperature in the convection zone between the individual iterations of the global linearization scheme. ICONRE has the meaning of the starting iteration number in which the correction is being calculated. However, the correction is performed only at depth points where the convective flux dominates over the radiative flux, the specific value is given by parameter CFRLIM. Usually, this routine helps significantly; there may however be cases when it does not help. The symptom of this is that the program produces essentially identical corrections of temperature in the linearization (that is, CONREF changes the temperature and the linearization changes it back). In those cases, routine CONREF should be disabled by setting ICONRE=0.
DEFAULT: ICONRE=1

CFRLIM – minimum local value of $F_{\mathrm{conv}}/F_{\mathrm{tot}}$ for which routine CONREF corrects the temperature in the convection zone.
DEFAULT: CRFLIM=0.7

If ICONRE is set to a positive value, then there are four additional parameters that control the work of routine CONREF, namely:

IDEEPC – if set to a positive value, then the correction to the current temperature is performed even in the so-called "convection gaps", which are defined as depth zones that are located between zones in which there is a convection ($\Delta > \Delta_{\mathrm{ad}}$), but for which the current values lead to $\Delta < \Delta_{\mathrm{ad}}$ and thus are viewed as convectively stable (this may happen during a global iteration process because in the convection zone Δ is always very close to Δ_{ad}, and the linearization may easily lead to Δ slightly smaller than Δ_{ad}).
– if IDEEPC=2 or larger, then if the convection zone ends at ND-1 depth zone, then it is reset to ND (ND being the total number of depth zones). Again, this may happen in the iteration process, and is essentially always spurious.
– if IDEEPC=3, then the end of convection zone is reset to ND regardless of where it currently ends.
– if IDEEPC=4, then if in the current iteration the end of convection zone appears above the beginning of the convection zone in the previous iteration, the current beginning and end are reset to the values from the previous iteration.
DEFAULT: IDEEPC=2

NDCGAP – specifies the number of the depth zones that define the "convection gap".
DEFAULT: NDCGAP=2

It is best to explain these parameters and corresponding computational strategies on an example. Let the convetion instability condition $\Delta > \Delta_{\mathrm{ad}}$ be currently satisfied for depth zones 10, 35-38, and 41-50. The convection at depth 10 is completely spurious, while the convection zone should extend from 35 to 50.

If IDEEPC is set to 0, then the convection zone is assumed to extend from depth 10 to 50, and the temperature correction is performed there. Since the algorithm forces the gradient to be close to the adiabatic one, this clearly leads to wrong results, and although linearization will try to correct temperature back, the routine CONREF with IDEEPC=0 would do more harm than help in this case.

If IDEEPC=1 or 2, and NDCGAP is set between 3 and 24, then the gap between 10 and 35 is too large to be considered a convection gap, and the extent of the convection zone is set correctly between depths 35 and 50. If NDCGAP is set to 1 or 2, then the gap between 38 and 41 is too large, and the temperature correction would be performed only between 41 and 50, so the convection zone would be spuriously narrow and the correction procedure would not work properly. This demonstrates that while NDCGAP should be set up to a reasonably large value, one should not set it to be too large. When code does not converge, one should inspect the standard output file where some details about temperature correction in the convection zone are provided, and which may give a clue as to what values of the convection switches to choose.

6.11   Parameters for a treatment of line blanketing

ISPODF - the basic mode of treating line blanketing:

= 0 - the Opacity Distribution Function (ODF) mode. Here, frequencies are set up for each line or ODF. ODFs cross-sections must be pre-tabulated; the filenames of the corresponding tables are specified in the standard input. In this case, there are no other optional parameters to be specified.

≥ 1 - the Opacity Sampling (OS) mode. Frequencies are set up systematically, with a variable step depending on lines and continua. Small frequency steps are adopted to sample adequately lines of light elements. In between these lines, iron-peak lines are sampled with a step DDNU times the fiducial Doppler with for Fe. Line cross-sections are calculated by TLUSTY based on Kurucz data files. Lines are selected dynamically based on a criterion including ionization, excitation and gf-value. Parameter STRLX sets the selection criterion (the smaller STRLX the more lines are selected; values $10^{-6} \leq$ STRLX $\leq 10^{-10}$ are generally appropriate). The cross-sections are recalculated after first 3 Ng accelerations if the maximum relative temperature change is larger than CHMAXT. Cross-sections are calculated by default (JIDS=0) at three depth points (top, bottom, and layer where $T \approx T_{\mathrm{eff}}$) and are logarithmically interpolated in between. They may be calculated at more depth points, in which case JIDS > 0 gives the number of layers.

Note: The default is set to 0 to help most new users to start with simple models (say, H-He only), with no lines or with a few lines, in which ISPODF=0 is appropriate. However, we stress that for computing fully blanketed models the option ISPODF=1 (the OS approach) is preferrable.

DEFAULT: ISPODF=0

DDNU - the step for Opacity Sampling expressed in fiducial Doppler widths for iron (see above).

DEFAULT: DDNU=0.75

CNU1 - Controls the highest frequency at which lines are taken into account (lines at higher frequencies are omitted). This frequency is defined as $\nu_{\mathrm{max}} = \mathrm{CNU1} \times 10^{11} \times T_{\mathrm{eff}}$. Frequencies for Opacity Sampling are set up from ν_{max} to lower frequencies, or from the highest bound-free limit if this limit exceeds ν_{max}.

DEFAULT: CNU1=4.5

CNU2 - Defines the lowest frequency for Opacity Sampling (lower frequencies are only included to represent the continuum and lines from light elements down to frequency `FRLMIN`. This lowest frequency is defined as $\nu_{\min} = 3.28805\,10^{15}/\mathtt{CNU2}^2$.
DEFAULT: CNU2=3.

STRLX - selection criterion for iron-peak elements lines in the Opacity Sampling mode (see above)
DEFAULT: STRLX=1.e-10

STRL1, STRL2 - Define groups of intermediate and weaker lines that will be represented by a limited number of frequencies, hence optimizing the number of frequencies in Opacity Sampling mode. DEFAULT: STRL1=0.001; STRL2=0.02

JIDS - number of depths at which the cross-sections for iron-peak (super)lines are computed.
= 0 - sets the default of 3 depths (ID=1, ND, and the depth where $T \approx T_{\mathrm{eff}}$);
> 0 - number of depths.
DEFAULT: JIDS=0

6.12 Non-standard atomic transition rates; hydrogen line profiles

There are two types of parameters here. First, there are parametgers that switch some otherwise non-included transition processes, like dielectronic recombination, charge transfer reactions, and collisional excitation/deexcitation by hydrogen atoms (in addition to transitions induced by electrons). Dielectron recombination, if switched on, is treated using the data from Aldrovandi & Pequignot (1973), Nussbaumer & Storey (1983), and Arnaud & Raymond (1992). Numerically, the procedure described by Hubeny et al. (2001 – Appendix B) is used that treats dielectronic recombination by introducing an artificial modification of the photoionization cross-sections. We also include in this category a global switch for setting up the default calculation of the hydrogen collisional excitation rates, ICOLHN.

The second category of switches is designed to provide more options to treat hydrogen line braodening. We will describe the parameters of both categories in turn.

IFDIEL – a global switch for dielectronic recombination.
= 0 – dielectronic recombination is neglected;
$\neq 0$ – dielectronic recombination is considered the procedure and data mentioned above.
DEFAULT: IFDIEL=0

IFCHTR – a global switch indicating that all the charge transfer reactions of neutral or ionized atoms (atomic number 2 to 30) with hydrogen are switched on. The charge transfer reaction is treated as an collisional transition from the ground state of an atom (neutral or ionized) to the ground state of the next ionization stage. We employ an appropriately modified routine written originally Kingdon and Ferland. One can also set up charge transfer for individual species separately by appropriately modifying parameter ICOL (see Sect.8.2).
= 0 – charge transfer is not set globally
$\neq 0$ – charge transfer set globally to all species with atomic number between 2 and 30 (He to Zn). In this case, charge transfer reaction are considered up to IFCHTR-1 times ionzed atoms; that is IFCHTR=1 means that the charge transfer reactions are switched on for neutral atoms only, IFCHTR=2 switched charge transfer for neutrals and once-ionized atoms, etc.
DEFAULT: IFCHTR=0

SHFAC — a global switch and multiplicative parameter for collisional excitation due to hydrogen atoms, after Drawin's original treatment generalized by Steenbock and Holweger (1984), with an empirical multiplicative factor given by SHFAC
= 0 – the process in neglected;
> 0 – value of an empirical factor that multiplies the Steenbock-Holweger formula.
DEFAULT: SHFAC=0.

ICOLHN – a switch for setting up the default calculation of the hydrogen collisional rates. We stress that setting this parameter to 1 or 2 will overwrite an evaluation of collisional rates specified by input parameter ICOL (coded in the input file for individual ions – see§8.3).
= 0 – hydrogen collisional rates are evaluated according to the values of ICOL.
= 1 – hydrogen collisional rates are evaluated using the data of Przybilla & Butler (2004) (for lines with the upper level up to $n = 7$; = 2 – hydrogen collisional rates are evaluated using the data by Giovanardi et al. (1987) (for lines with the upper level up to $n = 15$.
DEFAULT: ICOLHN=1

There are two different types of refinements for the hydrogen line broadening: considering the quasi-molecular satellites of Lyman α and β, and detailed hydrogen line broadening using Lemke (1997) tables.

IQUASI – switch for including quasi-molecular satellites
= 0 – quasi-molecular satellites are not included;
> 0 – quasi-molecular satellites are included. In this case one has to specify additional parameters NUNALP and NUNBET (see below).
DEFAULT: IQUASI=0

NUNALP – the unit number where the table of the absorption cross-section for the quasi-molecular satellites of Lyman α is located.
DEFAULT: NUNALP=3

NUNBET – the unit number where the table of the absorption cross-section for the quasi-molecular satellites of Lyman β is located.
DEFAULT: NUNBET=0

IHYDPR – a switch for considering Lemke's tables for hydrogen line broadening.
= 0 – hydrogen line broadening is treated as before (an approximate Stark broadening after Hubeny, Hummer, & Lanz 1994);
> 0 – hydrogen line broadening is computed using Lemke's table. The user then has to have file `lemke.dat` in the current directory.
DEFAULT: IHYDPR=0

6.13 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=4

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

6.14 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.
= −1 – wind blanketing is not considered; moreover the incoming radiation is either exactly zero, or is set up through parameters TRAD and WDIL.
DEFAULT: IWINBL=-1 (no wind blanketing; no incoming radiation unless specified explicitly)

NRETC – a switch for setting an option of fixed temperature at the upper layers
= 0 – no fixed temperature; radiative equilibrium is solved for all depths
> 0 – the temperature at first NRETC depth points is held fixed (given by the input model); radiative equilibrium at those depths is not solved for.
DEFAULT: NRETC=0

XGRAD – a switch controlling an artificial lowering of radiation acceleration at surface layers.
= 0 – allows to auto-limit the radiative acceleration to some fraction of the gravity in the 10 uppermost depth points. The fraction of the gravity acceleration to which the radiation acceleration is limited to was found empirically and is hard-wired in the program; it is given as $(0.1, 0.3, 0.5, 0.7, 0.9, 0.92, 0.94, 0.96, 0.98, 0.99)$ times g, in the first 10 depths, respectively.
= −1 or −2 – allows to impose a more stringent cut-off in the 20 uppermost layers.
> 0 – auto-limits the radiative acceleration to fraction XGRAD of the gravity acceleration g *everywhere* in the atmosphere.
DEFAULT: XGRAD=0.

6.15 Parameters determining an amount of additional output

IPRIND – if set to a non-zero value, a condensed model atmosphere is stored after each iteration of complete linearization (Unit 17) – see Sect.10.2
DEFAULT: IPRIND=0

ICOOLP – if set to a non-zero value, the net total cooling rate is stored as a function of depth (Unit 86); if moreover it is set to a vale > 10, also the individual cooling rates for all explicit ions are stored (Unit 87) – see Sect.10.2.
DEFAULT: ICOOLP=0

ICHCKP – if set to a non-zero value, an additional output showing the total transition rates in and out of all explicit levels is generated (Unit 16) – see Sect.10.2.
DEFAULT: ICHCKP=0

IPRINP – if set to a non-zero value, the explicit level populations are stored in output unit 7 (condensed model atmosphere) even for LTE models (the populations are always stored for

a NLTE model, so in NLTE this parameter has no effect).
DEFAULT: IPRINP=1

IPOPAC – if set to a non-zero value, an additional output of opacity for all continuum frequencies as a function of depth is generated (Unit 85)
DEFAULT: IPOPAC=0

6.16   List of all optional parameters in alphabetic order

Here we give the list of all optional parameters in alphabetic order, including their default values, and the reference for the section they are described in.

ABPLA0	0.3	6.3
ABPMIN	10^{-5}	6.3
ABROS0	0.4	6.3
ALBAVE	0	6.3
ALPHAV	0.1	6.1
CFRMAX	2 (0 for disks)	6.2
CHMAX	10^{-3}	6
CHMAXT	0	6.7
CNU1	4.5	6.11
CNU2	3	6.11
CRFLIM	0.7	6.10
DDNU	0.7	6.11
DFTAIL	0.25	6.2
DION0	1.	6.3
DJMAX	0.001	6.5
DM1	10^{-3}	6.3
DMVISC	0.01	6.1
DPSILD	1.25	6.7
DPSILG	10.	6.7
DPSILD	1.25	6.7
DPSILN	10.	6.7
FRACTV	-1	6.1
FRCMAX	0.	6.2
FRCMIN	10^{12}	6.2
FRLMAX	0.	6.2
FRLMIN	10^{13}	6.2
HCMASS	0	6.1
HMIX0	-1.	6.1
IACC	7	6.13
IACD	4	6.13
IACDP	4	6.6
IACPP	7	6.6
IATREF	1	6.6
IBC	3	6.5
IBFINT	1	6.7
IBPOPE	1	6.7
ICHANG	0	6.4

ICHC	0	6.6
ICHCKP	0	6.15
ICOLHN	1	6.12
ICONRE	1	6.10
ICONV	0	6.10
ICOOLP	0	6.15
IDEEPC	2	6.10
IDGREY	0	6.3
IDLST	5	6.8
IDLTE	1000	6.6
IELCOR	100	6.6
IFALI	5	6.5
IFCHTR	0	6.12
IFDIEL	0	6.12
IFIMXO	0	6.8
IFLEV	0 for NLTE; 1 for LTE	6.6
IFPOPR	4	6.6
IFPREC	1	6.6
IFRALI	0	6.5
IH2	0	6.3
IH2P	0	6.3
IHECOR	0	6.7
IHM	0	6.3
IHYDPR	0	6.12
ILASCT	0	6.5
ILDER	0	6.7
ILMCOR	1	6.5
ILPSCT	0	6.5
INDL	0 (3 with convection)	6.8
INHE	1	6.8
INMP	0	6.8
INPC	3 (4 with convection)	6.8
INRE	2	6.8
INSE	4 (5 with convection)	6.8
INTRPL	0	6.4
IOPADD	0	6.9
IOPH2P	0	6.9
IOPHE1	0	6.9
IOPHE2	0	6.9
IOPHMI	0	6.9
IOVER	1	6.7
IPOPAC	0	6.15
IPRESS	0	6.10
IPRIND	0	6.15
IPRING	0	6.3
IPRINP	0	6.15
IPRINT	0	6.10
IPTURB	1	6.1

IQUASI	0	6.12
IRDER	3	6.7
IRSCT	0	6.9
IRSPLT	1	6.6
IRTE	3	6.5
ISPLIN	0	6.5
ISPODF	0	6.11
ITEK	4	6.13
ITEMP	0	6.10
ITGMAX	10	6.3
ITLAS	100	6.7
IVISC	0	6.1
IWINBL	-1	6.14
IZSCAL	0	6.1
JALI	1	6.5
JIDS	0	6.11
MLTYPE	1	6.1
MODREF	1	6.6
NCONIT	10	6.3
ND	70	6.7
NDCGAP	2	6.10
NDGREY	0	6.3
NDRE	0	6.8
NELSC	0	6.7
NFTAIL	21	6.2
NITER	30	6.7
NITZER	3	6.6
NLAMBD	2 (1 for LTE)	6.7
NLAMT	1	6.5
NMU	3	6.5
NNEWD	0	6.3
NRETC	0	6.14
NTRALI	3	6.5
NUNALP	3	6.12
NUNBET	0	6.12
ORELAX	1.	6.13
POPZER	10^{-30}	6.6
POPZR2	10^{-30}	6.6
RADSTR	0	6.1
RADZER	10^{-20}	6.6
SHFAC	0	6.12
STRL1	0.001	6.11
STRL2	0.02	6.11
STRLX	10^{-10}	6.11
TAUDIV	0.5	6.8
TAUFIR	10^{-7}	6.3
TAULAS	316.	6.3
TDISK	0	6.3

TRAD	0.	6.1
TSURF	0.	6.3
VTB	0.	6.1
XGRAD	0.	6.14
WDIL	1.	6.1
ZETA0	0.	6.1
ZETA1	0.	6.1

7 SUMMARY OF NUMERICAL AND PHYSICAL TRICKS

TLUSTY introduces a variety of numerical and physical tricks that aim at speeding up calculations, avoiding convergence problems, or introducing minor physical simplifications that do not deteriorate the quality of the resulting model. All such tricks prove useful in some cases, but in some other cases they may harm the convergence or even yield to additional numerical problems.

Most of keyword parameters that switch on/off such options are set as default values and may be changed by setting an appropriate value in the optional flags file. The choice of defaults was made based on experience gained from many different models, and typically a default value was found successful in most cases. However, there are cases where those default values may be changed to improve the convergence properties of the run.

We will summarize the tricks and their appropriate control keyword(s), together with a brief discussion, below. We stress that we described here only computational options. Obviously, the model atmosphere itself as well as its convergence properties may be significantly influenced by the global choice of explicit species, energy levels, and general atomic data. The topic of atomic data and their choice is discussed in detail in Sect. 8

The following text will present an explanation of many optional keyword parameters introduced above. The previous chapter presented a formal explanation; the present one will concentrate more on practical aspects, in particular on the role of the individual parameters in troubleshooting and dealing with convergence problems.

There are essentially four categories of such parameters; i) flags for switching purely numerical tricks: ii) parameters that influence an accuracy of the model; iii) parameters that introduce minor, but helpful physical approximations; and iv) parameters that switch on/off a potentially important, but still optional, physics. We will discuss these categories in turn.

7.1 Purely numerical tricks

These procedures are defined such as their use does not change the resulting model. In other words, using or not using an option, provided that both options converge, would lead to the same numerical results (that is, essentially the same results; the rounding errors and other computer-related inaccuracies may lead to differences at 4th and higher decimal place of the computed model parameters.

- *Set-up of of the hybrid CL/ALI scheme*
  This is partly set up by the atomic data files, where one uses default settings – the first six frequencies in the hydrogen Lyman continuum; the three central frequencies in the Lα, and the central frequency in Lβ and Lγ, together with first three points in the He II Lyman continuum are set to linearized mode; the rest of frequencies is in the ALI mode.
  There is also a useful keyword IFRALI (see Sect. 6.5) which can change the setup globally.

- *Accelerations*

  There are two accelerations, Ng and Kantorovich. The corresponding keywords are described in Sect.6.13. Both accelerations are helpful tools to speed up calculations considerably, or even sometimes to improved convergence properties, but on the other hand they may cause problems in some cases. Therefore, they should not be used blindly.

  One should be careful about the parameter IACC, which represents the iteration number where the Ng acceleration is done for the first time. If the value is too low, the acceleration is done too soon, with a consequent harmful or disastrous effect upon the convergence; if it is done too late it didn't do what it could have, namely speed up the calculations. In some cases the Ng acceleration is even crucial for the success of the run; it is when the normal linearization produces a regular oscillations, so that only Ng acceleration is able to find the way out of otherwise non-convergent situation. The best strategy is to examine carefully the convergence log (file `fort.9`); if the convergence pattern deteriorates drastically exactly at the iteration number when Ng acceleration was switched on, a simple cure is to increase the value of `IACC`. If, in contrast, one sees an oscillatory behavior for many iterations, and just at the onset of Ng acceleration the maximum change suddenly drops, it is advisable to try to decrease the value of `IACC`.

  In the case of convection, Ng acceleration may often be harmful; in this case one may skip the acceleration completely, i.e. to set IACC to a value larger than NITER.

- *Level grouping*

  This numerical trick may significantly reduce the number of level populations to be linearized. The level group is a set of one or more levels whose populations are assumed to vary in a coordinated way in the linearization. More precisely, instead of linearizing the individual level populations, one linearizes the total populations of the groups, assuming that the ratios of the individual level populations within the group to the total population of the group is unchanged in linearization. In the formal solution step, one solves exactly for all the individual level populations. The concept of level groups should not be confused with the concept of superlevels; in the former case, the level groups are only a numerical trick to make the matrices of complete linearization smaller, while the level populations are determined exactly; the latter case – superlevels – approximates the individual populations of the components of the superlevel by assuming that they are in Boltzmann equilibrium with respect to each other. In fact, one may group the individual superlevels into level groups as well.

  The grouping is set up by the atomic data files (parameter IMODL; see Sect. 8.1). The standard files, for instance those distributed through the TLUSTY website, contain a default level grouping. This grouping works well in most cases. However, the user should be aware that under some circumstances (e.g., low temperature), this grouping may cause convergence problems, and should be reset by changing parameter IMODL, typically by letting more low-lying levels to form a single-level group.

- *Choice of radiative transfer formal solver*

  This is driven by keyword ISPLIN (see Sect. 6.5). Usually, the original 2nd-order Feautrier scheme (ISPLIN=0; the default) works very well. The only exception is a case of strong external irradiation; in this case setting ISPLIN=5 (the DFE scheme) may be preferable.

- *Number of internal "Lambda" iterations in the formal solution*

  This is driven by keyword NLAMBD. The default value (NLAMBD=2) usually works well; in some cases one may increase this number, which increases the computer time, but may provide a more stable scheme.

- *Choice of the approximate Λ^*-operator*
  This is driven by keywords IFALI (see Sect. 6.5) – diagonal or tridiagonal operator, and JALI (Rybicki-Hummer or Olson-Kunasz evaluation). While the value of JALI usually does not matter, in some cases a tridiagonal operator (set up with IFALI=6 - notice that the default is IFALI=5, corresponding to the diagonal operator) may provide a more stable solution. However, at present, this option is not yet fully tested, and may not work properly in some cases.

- *Choice of treatment of the approximate Λ^*-operator at the lower boundary*
  This is driven by keyword IBC (see Sect. 6.5). Usually, the default value works well.

- *Choice of the so-called "reference atom" and "reference levels"*
  This is driven by keyword IATREF and MODREF (see Sect. 6.6). Usually, the default values work well. However, for highly unusual chemical compositions, in particular for extremely hydrogen-deficient objects, it is advisable to set IATREF=2 (so that He will be the reference species).

- *Treatment of charge conservation in the formal solution*
  This is driven by keyword IELCOR (see Sect. 6.6). Usually, the default value works well.

- *Choice of treatment of electron scattering with the hybrid CL/ALI approach*
  This is driven by keywords ILMCOR, ILPSCT, and ILASCT (see Sect. 6.5). Usually, the default values work well.

- *Limiting the values of the relative changes to be used to obtain next iterates of structural parameters*
  This is driven by keywords DPSILT, DPSILG, DPSILN, DPSILD - see Sect. 6.7. Usually, the default values work well.

7.2 Change of parameters that influence the accuracy of the model

In this category there are parameters that are originally meant to influence an accuracy of the model without significantly changing its general properties (e.g., the number of depth points). However, these parameters may in certain cases significantly influence the global convergence properties.

- *Number of depth points*
  The default value (ND=70) is usually satisfactory. In some cases (for instance if some quantities vary very sharply with depth), it may be helpful to increase this value. On the other hand, for hot stars it is highly recommended to decrease the value to ND=50, which saves computer time without a decrease of the accuracy of the model (in fact, this was used in our recent O-star model grid calculations - Lanz & Hubeny 2003).

- *Setting up the minimum and maximum Rosseland optical depth for a model* (only if the model is computed from scratch)
  This is driven by keywords TAUFIR and TAULAS (see Sect. 6.3). The default values usually work well; in special cases one may need to increase TAULAS or to decrease TAUFIR. For instance, to produce X-ray spectra of, say, a DA white dwarf, one has to set TAULAS to a very large value ($\approx 10^4$ or m) because hydrogen provides very little opacity in the X-ray region and thus the atmosphere is very transparent there.

- *Convergence criterion*

  Driven by keywords NITER and CHMAX (see Sect. 6.7). We recall that NITER represents the maximum number of the global linearization iterations. If set to zero, the program only computes radiation field and prints an output information. This is useful if for instance some output files of the previously computed model (but not the resulting model file on unit 7) were accidentally destroyed; or for some exploratory calculations to test a basic setup without a goal to produce a converged model.

- *Treatment of the iron-peak lines* This is controlled by keywords ISPODF, DDNU, STRLX, CHMAXT, and JIDS - see Sect. 6.11. These parameters influence typically an accuracy of the model (and, obviously, the computer time needed to generate a model), but usually not its convergence properties.

7.3 Tricks that introduce helpful minor physical approximations

Here, we introduce physical approximations that either shorten the computer time, or help to prevent convergence problems. In some cases, these tricks lead to negligible deficiencies in the computed model; in some cases (e.g. rejecting, i.e. setting to detailed radiative balance, of too many lines) would provide a model of an insufficient accuracy. In such a case, the option is useful to compute an intermediate model, starting from which one may compute a more realistic model that would not converge otherwise.

From the point of view of troubleshooting, the following parameters are the most important ones, so this Section warrants a careful reading.

- *Division point between differential and integral treatment of the radiative equilibrium*

  This is driven by keywords TAUDIV, IDLST, and NDRE – see Sect.6.8. The most important parameter is TAUDIV – the division point for treating energy balance as a linear combination of the differential and integral form (see Hubeny & Lanz 1995). Changing this value is often *the* decisive trick to make LTE models converge. There is no a priori recipe which value is the best, or whether to increase or decrease it. The most reasonable strategy is to try two values of both sides of the default (which is 0.5), say 0.05 and 5 or so. Experience shows that for cool stars ($T_{\mathrm{eff}} < 10,000$ K) setting TAUDIV=5 usually helps. In contrast, for accretions disks the value TAUDIV=0.05 is sometimes advantageous. However, the user should be aware of the fact that this trick may lead to numerical inaccuracies – when the linear combinations of the differential and integral equations from is satisfied, this does not necessarily mean that both are satisfied individually. The errors are the larger the higher the value of TAUDIV is set. If the user sets a value larger than the default, is is advisable to recompute the converged model with a default value of TAUDIV. In other words, increasing TAUDIV to obtain an intermediate model may enable to converge model that would not converge directly with the default value of TAUDIV.

- *Artificial lowering of the total radiative pressure at the surface*

  Radiative acceleration increases in superficial layers ($\tau_{\mathrm{Ross}} < 10^{-5}$), and may overcome the gravitational acceleration. The model may become numerically unstable in these layers, although physically stable at larger optical depths. Option XGRAD=0 allows to auto-limit the radiative acceleration to some fraction of the gravity in the ten most upper points. This is the default value. XGRAD=-1., or -2., allows to impose a more stringent cut-off in the 20 most upper layers, which may critically help convergence near the Eddington limit. XGRAD > 0 auto-limits the radiative acceleration to fraction XGRAD of the gravity acceleration

g everywhere in the atmosphere. Potentially, this may lead to an incorrect atmospheric structure, so this option may be used only with extreme caution.

- *Fixed temperature at a surface layer*
  This is set up by the parameter NRETC (see Sect. 6.14). The option is useful if the model does not converge at the upper layers, while the convergence is reasonable elsewhere. In this case one may set up, for instance, NRETC=10 (that is, the temperature at first 10 depth points will be held fixed to the values given by the input model). Once one obtains a converged solution, it is recommendable to reconverge the model with NRETC=0 (the default), i.e. with the radiative equilibrium solved exactly at all depths.

- *Setting up the minimum and maximum frequency*
  This is driven by parameters FRCMIN and FRCMAX – see Sect. 6.2. In some cases it may be advantageous to obtain an intermediate model by lowering the maximum frequency FRCMAX, because high frequencies may cause numerical problems due to high sensitivity of mean intensities to the state parameters, in particular to temperature.

- *Setting up frequency points in a high-frequency tail*
  This is driven by parameters NFTAIL, DFTAIL, and CFRMAX - see Sect. 6.2. The default values usually work well; in some cases, typically with Comptonization (i.e. for very hot atmospheres or, in particular, disks), one may consider more frequencies in the high-energy tail, that is increasing NFTAIL.

- *Setting a detailed balance in lines*
  In many cases, this trick helps to provide an intermediate model if other tricks fail. One may set up a detailed radiative balance in a line (and therefore to exclude the corresponding transition rate from the statistical equilibrium equation, and removing the corresponding opacity) in several different ways:
  i) individually; in which case one has to modify the corresponding entry in the atomic data file (see Sect. 8.3). This is the most flexible way, but also most cumbersome since one has to modify the atomic data file.
  ii) excluding all lines of an atom/ion that originate from a selected set of lower levels. This is driven by the parameter ILVLIN (see Sect. 5.4) for a given atom/ion, coded in the standard input. The meaning of ILVLIN is that all lines originating at level index lower than ILVLIN are set up to detailed radiative balance. For instance, ILVLIN=2 excludes all resonance lines (i.e., originating from the ground state with index 1); setting ILVLIN=99 (or some other large number) will effectively set all lines of the given atom/ion to detailed balance. Traditionally, such an approach was often used as an intermediate NLTE model, usually called NLTE/C (continua-only) model. The ALI method will often allows the uses to converge a full NLTE model with all lines directly from a starting LTE model, so that converging first a NLTE/C model is no longer a mandatory option, though still usefull in some difficult cases.
  iii) The third way to set lines to detailed balance is based on their wavelength (frequency). This is driven by optional parameters FRLMAX and FRLMIN (see Sect. 6.2), which set all lines with frequency smaller than FRLMIN and/or larger than FRLMAX to detailed balance. Setting FRLMIN to values around 10^{13} will not only save computer time because it excludes all far-infrared lines that typically do not influence the atmospheric structure, but also remove possible problems with laser effect in lines, which may lead to numerical problems.

- *Level zeroing*
  This is a useful trick that may avoid some floating-point problems. The idea is as follows:

Whenever a local population of a level becomes lower than a prescribed fraction of the total population of the species (given by the parameter POPZER; with a default value 10^{-30}), the population is set exactly as zero, and instead of considering an appropriate rate equation for such a level, one replaces it by a simple condition $n_i = 0$. This does not decrease the number of state parameters, but improves numerical stability without compromising the final solution.

- *Zeroing of the mean intensity*
  Analogously, one may set the mean intensity of radiation to zero if the value of the mean intensity decrease below a prescribed fraction of the maximum mean intensity. This fraction is given by the optional parameter RADZER, with a default value 10^{-20}.

- *Keeping selected structural parameters fixed*
  This is driven by keywords described in Sect.6.8. Any of these options may be useful to compute an intermediate model in cases when convergence cannot be achieved with all structural parameters being linearized. Usually, keeping just temperature fixed (INRE=0) will provide an intermediate converged model; in some cases it is better to keep also electron density and the total particle density fixed; in this case one may code the shortcut parameter IFIXMO=0.

7.4 Potentially important, but still optional, piece of physics

This category of trick contains removing or including a major physical mechanism (e.g. convection, Compton scattering, etc.) that should be either present always, or should be uniquely given by the considered model parameters, but are left to the discretion and judgment of the user whether they are included or not. The reason is that at the intermediate case between a completely negligible and almost negligible influence of the given mechanism its inclusion or rejection may significantly influence convergence properties of the model.

- *Convection*
  Parameters for switching on and treating convection are described in Sects. 6.1 (HMIX0, MLTYPE), and 6.10 (ICONV, IPRESS, ITEMP). If the convection is weak, it may be advantageous to converge first a model without convection; sometimes it is however better to include convection from the outset. There may still be problems for very cool stars; we are working on a more robust scheme for treating convection.

- *Additional opacity sources*
  This is driven by parameters IOPADD, IRSCT, IOPHMI, IOPH2P – see Sect. 6.9. This option was useful in the past where only a limited amount of explicit atoms, ions, and levels could be considered. The utility of the so-called additional opacities is lower now, but there are still cases where it is useful. For instance, one may simply switch on a H^- opacity even if the H^- ion is not an explicit ion (however, treating H^- as an explicit ion is preferable because this approach can account for NLTE effects in H^-). Another example is the Rayleigh scattering opacity (IRSCT), or H_2^+ opacity (IOPH2P). In the two latter cases, setting IRSCT and IOPH2P to non-zero values is the only available mechanism in TLUSTY how to switch on these opacities.

- *Compton scattering*
  Compton scattering is important for very hot atmospheres and, in particular, accretion disks. It is switched on by set up parameter ICOMPT to a non-zero value.

- *Microturbulence and turbulent pressure*
  This is driven by parameters VTB and IPTURB – see Sect. 6.1. The value of VTB does not usually influence the convergence properties of the model. On the other hand, parameter IPTURB, which decides whether the assumed microturbulence will will be associated with a corresponding turbulent pressure, and thus influence the hydrostatic equilibrium. In case of a high microturbulence (close to, or larger than, the thermal velocity), a safer and perhaps more physical setting is to set IPTURB=0, in which case there is no turbulent pressure associated with an assumed turbulent velocity.

8 INPUT FILES FOR THE INDIVIDUAL IONS

The input file contains information about three or four basic types of atomic data (the fourth type is only required in the OS mode), 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).

4. Energy bands for setting superlevels of iron-peak elements (only required in the OS mode)

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. In fact, such a library is available through the TLUSTY website, `http://nova.astro.umd.edu`.

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.

`****** Energy bands`

followed by limits for energy bands for superlevels, without any comment line.
We will now describe the three basic blocks of the ionic input file in detail.

8.1 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 – a mode of the treatment of level dissolution (See Hubeny, Hummer, & Lanz 1994):
$= 0$ – occupation probability set to 1, i.e no level dissolution;
$= 1$ – occupation probability of the level is calculated, and is used consistently in the rate equations and in evaluating the opacities and emissivities;
$= 2$ – depth-dependent statistical weight for the iron-peak superlevels is calculated (see Hubeny & Lanz 1995).
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 There are several options, which all are more or less outdated. The only practical use of parameters IMODL is to set up the *level groups*. The level group is a set of one or more levels whose populations are assumed to vary in a coordinated way in the linearization. More precisely, instead of linearizing the populations of the individual levels, one linearizes the total population of the groups, assuming that the ratios of the individual level populations within the group to the total population of the group is unchanged in linearization. In the formal solution step, all the individual level populations are solved for exactly. The concept of level groups should not be confused

with the concept of superlevels; in the former case, the level groups are only a numerical trick to make the matrices of complete linearization smaller, while the level populations are determined exactly; the latter case – superlevels – approximate the individual populations of the components of the superlevel by assuming that they are in Boltzmann equilibrium within each other. In fact, one may group the individual superlevels into level groups as well.

$= 0$ – the level is linearized (i.e., it forms its own group);

< -100 – the given level is a member of a level group. A group is this defined by all levels with the same value of IMODL. For instance, all levels with IMODL$=-101$ will from one group; the levels with IMODL$=-102$ another group, etc. It is usually advisable to form the level groups by levels with the same multiplicity and parity. The actual value of parameter IMODL is inconsequential.

8.2   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 – relative index of the lower level (i.e. II=1 corresponds to the ground state, etc.)

JJ – relative 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 1):
$= 0$ – 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 1 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 1;

$= 3$ – the so-called SIMPLE2 mode - see Appendix 1;

> 10 – the collisional rates contains also a contribution from the charge transfer reaction. ICOL-10 has then the meaning of the regular mode ICOL for setting the evaluation of the true collisional ionization rate. We note that even if ICOL is set to a value below 10, charge transfer may still be switched on by setting the non-standard parameter IFCHTR (see Sect.6.12) to a positive value.

< 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 1 for details);

CPARAM – second collision parameter (see Appendix 1 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 1 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.

8.3 Parameters for bound-bound transitions

The structure is analogous to that for the bound-free transitions, § 8.2. 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 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 – in the OS mode, TLUSTY computes the detailed line cross-sections from the basic atomic data; in the ODF mode, the ODF is calculated by a separate program, and is communicated to TLUSTY by means of two additional input files (see § 5.5).
$= 9$ 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).
This option is obsolete! Use instead the XGRAD keyword, see Sect. 6.14 and 7.3).
> 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 a spurious overlap of a normal and an ODF line). With the OS approach, this option is obsolete.

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;

= 3 or −3 – hydrogen line profiles given by Lemke's tables. However, if the keyword parameter IHYDPR is set to a non-zero value, the Lemke's profiles are switched on globally and the program resets the IFANCY for appropriate transition automatically, so they do not need to be modified by hand.

≥ 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 1.

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

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

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

= 2 – the so-called SIMPLE1 mode – see Appendix 1;

= 3 – the so-called SIMPLE2 mode – see Appendix 1;

= 4 – Eissner-Seaton formula - see Appendix 1;

= 5 – Van Regemorter formula for neutral atoms – see Appendix 1;

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 1 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. Again, it is obsolete in the OS option.

(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 among 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; which is the default), all lines are set by default to the full-profile mode. Therefore, 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;
= 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. $\Gamma = -\mathtt{STARK1} \times \Gamma^{\mathrm{clas}}$, where $\Gamma^{\mathrm{clas}} = 10^{-8}\, n_{\mathrm{eff}}^{5/2}\, n_{\mathrm{e}}$, where n_{eff} is the effective quantum number of the upper level;

> 0 – Stark broadening given by $n_{\mathrm{e}}\,(\mathtt{STARK1} \times T^{\mathtt{STARK2}} + \mathtt{STARK3})$, where $\mathtt{STARK2,}$ $\mathtt{STARK3}$ 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.

8.4   Energy bands for superlevels

Finally, data files for iron-peak elements must provide the limits of energy bands used to built the superlevels, first for even-parity levels, then for odd-parity. This is required only in OS mode where TLUSTY reads detailed lists of individual energy levels from Kurucz files and construct the superlevels. This list of energy bands must be consistent with the level data given at the top of the file.

8.5   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
3.24D15                         ! Lyman pseudocontinuum extends to nu=3.24D+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 $\sigma_0 = 5.006 \times 10^{-19}$ – 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 therefore $2 \times 7 - 1$, i.e. 13. The index of the core frequency is 7.

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.

9 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. 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.

9.1 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 (or 4 for disks) – for LTE model;
> 3 (or 4 for disks) – 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})

ZD – geometrical distance from the midplane (cm) – for disks only

level populations – needed only for a NLTE input model (but populations can be present for an LTE model, although they will be immediately recomputed). Number of input level populations need not be equal to NLEVEL; in that case ICHANG 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.

9.2 Change of the input level structure

The change of the explicit level structure is controlled by parameter ICHANG – see § 6.4. If this parameter is coded negative, 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

9.3   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 if 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, the optional parameter ND should be set to 63 (i.e. ND=63 should appear in the optional parameter file (see § 6.7).

10   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. TLUSTY does not contain any explicit OPEN statements for the output files, so the files are generated with names fort.nn, where nn is the corresponding unit number.

1. Basic output, generated always

    - Unit 6 – Standard output
    - Unit 7 – Condensed model atmosphere
    - Unit 9 – Convergence log
    - Unit 10 – Performance and error log
    - Unit 12 – b-factors (NLTE departure coefficients)
    - Unit 13 – Emergent flux in all frequency points
    - Unit 18 – Convergence log for formal solution
    - Unit 69 – Timing log

2. Auxiliary output, generated only if required (by setting corresponding optional parameters – see Sect. 6.15)

    - Unit 14 – Emergent (angle-dependent) specific intensities in all frequency points (at present implemented only in case of Compton scattering)
    - Unit 16 – Check of the statistical equilibrium equation solution
    - Unit 17 – Condensed model atmosphere in every iteration
    - Unit 85 – Opacities for all continuum frequencies
    - Unit 86 – Total and net cooling rates
    - Unit 87 – Net cooling rates separately for all ions

10.1 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.

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 the same unit 5; one only needs to specify NITER=0 in the optional parameters file.

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.

The file is generated after each set of formal solutions before entering a next iteration of the complete linearization, and is always overwritten so that only the quantities at the last completed iteration are stored.

Unit 12: b-factors.

The file is exactly analogous to the Unit 7 output file; only instead of populations the file contains the b-factors (NLTE departure coefficients).

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 `PCONV` 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, given by the optional parameter CHMAX (10^{-3} being a reasonable value in most cases).

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 13 – Emergent flux.

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

FREQ – value of frequency (in s^{-1})

FLUX – emergent flux, precisely the first 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

Note: In versions prior to version 200, additional quantities were printed out in this file.

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 69: Timing.

As pointed out above, this file is produced only under Unix or Linux (and NOT in Mac OSX). 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 the line calling the routine TIMING, and at all lines of this routine. 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.

10.2 Auxiliary output

Unit 14 – Angle-dependent emergent specific intensities

This file is generated only in the case of Comptonization, i.e. if ICOMPT > 0.

Unit 16 – Check of the statistical equilibrium

This output is generated only if the optional parameter ICHCKP is set to a non-zero value.

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 thus contain much lower values than the previous two columns. Generated by subroutine CHCKSE in the final iteration.

Units 17 and 20 – condensed models in each iteration

This output is generated only if the optional parameter IPRIND is set to a non-zero value.

These files are completely analogous to Unit 7 and 12 outputs, respectively; the only difference being that the values for all completed iterations are stored. These files can be used to recover partially converged models in case the final models crashed or diverged due to numerical reasons (e.g., an improper use of acceleration techniques, etc.).

Unit 85 - opacities in the continuum frequencies

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This output is generated only if the optional parameter IPOPAC is set to a non-zero value.

The file contains NFREQC (the number of frequency points in the continuum) blocks; each block contains data for one frequency point. The block contains first the frequency index and the value of frequency (Hz), then ND values of opacity (per gram) for all depth points, ID= $1, \ldots$,ND. Frequencies go from the highest to the lowest.

Units 86 and 87 - cooling rates

This output is generated only if the optional parameter ICOOLP is is set to a non-zero value.

Unit 86 contains four columns; the depth index, the total net cooling rate without an influence of scattering (C_{net}), the total net cooling rate including scattering (C'_{net}), and the total cooling rate (i.e., the true radiative cooling – without a balancing effect of radiation heating, C_{tot}). The two net cooling rates are identical in the case of coherent scattering (e.g. Thompson limit of electron scattering); but are generally different for non-coherent scattering (Compton).

$$C_{\mathrm{net}} = 4\pi \int_0^\infty (\eta_\nu - \kappa_\nu J_\nu) d\nu \,,$$

$$C'_{\mathrm{net}} = 4\pi \int_0^\infty (\eta_\nu + \sigma_\nu J_\nu - \chi_\nu J_\nu) d\nu \,,$$

$$C_{\mathrm{tot}} = 4\pi \int_0^\infty \eta_\nu d\nu \,,$$

where η_ν is the thermal emission coefficient; κ_ν the (thermal) absorption coefficient, χ_ν the total extinction (absorption + scattering) coefficient, all at frequency ν.

It IPRINP is set to a value larger than 10, an additional output is generated – Unit 87 – that contains the cooling rates separately for all explicit ions.

Acknowledgements

APPENDIX 1 – 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` $\leq$ 0 : standard expressions from Mihalas et al. (1975).

Other elements:

Ionization:

- for `ICOL` $= 0$: $\Omega = 1.55 \times 10^{13} T^{-1/2} U_0^{-1} \exp(-U_0) \sigma_0 \bar{g}$, $\quad \bar{g}\sigma_0 \equiv$ `OSC` (Seaton's formula)
  where $\bar{g} = 0.1$ for neutral atoms, $\bar{g} = 0.2$ for singly ionized atoms, and $\bar{g} = 0.3$ otherwise.

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

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

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

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

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

- for `ICOL` $= 1$: the same as above, but now $\bar{g}$ is an input parameter (`CPAR`) (van Regemorter formula). $\bar{g}$ should be taken $\bar{g} = 0.2$ for the transitions $nl \rightarrow n'l'$ (where $n \neq n'$), and $\bar{g} = 0.7$ for the transitions $nl \rightarrow nl'$.

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

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

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

- for `ICOL` $= 5$: $\Omega = 19.7363\, f_{ij}\, T^{-3/2}\, U_0^{-1} \exp(-U_0)\, \Gamma(U_0)$, $\quad$ where
  $\Gamma(U_0) = 0.276 \exp(U_0)\, E_1(U_0)$, $\quad$ for $U_0 \leq 14$, $\quad$ and
  $\Gamma(U_0) = 0.066\, U_0^{-1/2}\, (1 + 1.5 U_0)$, $\quad$ for $U_0 > 14$
  (Van Regemerter formula for neutral atoms);

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.

APPENDIX 2 – EQUATIONS OF ACCRETION DISKS

Classical disks

The disk is assumed in steady state, geometrically thin and in Keplerian rotation. The vertical structure is solved for a set of axially symmetric concentric rings where a plane-parallel 1-D atmosphere calculation is performed. The atmosphere at each disk radius R (specified in the disk midplane) is in hydrostatic equilibrium, with a depth-dependent gravity (g) that arises from the vertical component of the central star's gravitational force on the disk material. Neglecting the self-gravity of the disk and assuming that R is much larger than the distance from the central plane (z):

$$\frac{dP}{dz} = -g(z)\rho$$

$$g = \frac{GM_*z}{R^3}$$

where P is the pressure, ρ is the mass density, M_* is the central star mass, and G is the gravitational constant. The mass surface density is given by the standard disk model (Shakura & Sunyaev 1973):

$$\Sigma \equiv 2\,m_0 = \frac{\dot{M}}{3\pi\bar{w}} \left[1 - \left(\frac{R_*}{R} \right)^{1/2} \right]$$

$$\bar{w} = \frac{(GM_*R)^{1/2}}{Re}$$

where $\dot{M}$ is the mass transfer rate, $R_a st$ is the central star radius, and $\bar{w}$ is the depth-averaged kinematic viscosity, parametrized in terms of the Reynolds number Re of the flow (Lynden-Bell & Pringle 1974) and Kriz & Hubeny 1986). The viscosity w is allowed to vary as a power law of the mass column density above a certain physical depth $m(z)$:

$$w(m) = \bar{w}(\zeta + 1) \left(\frac{2m}{\Sigma} \right)^{\zeta}$$

The power law index ζ is usually set to a numerical value larger than zero to prevent the "thermal catastrophe" of the disk in the low optical depth regions where electron scattering is the dominant (only) opacity source (Hubeny 1990a).

The disk radiates all the mechanical energy dissipated by viscous shearing between the Keplerian orbits. According to standard formulae this quantity may be written as follows:

$$D_{\mathrm{mech}}(z) = \frac{9GM_*w(z)\rho(z)}{4R^3}$$

The energy balance equation then reads

$$\int_0^\infty (\kappa_\nu J_\nu - \eta_\nu)d\nu = D_{\mathrm{mech}}(z)$$

where κ_ν and η_ν are the absorption and emission coefficient, and J_ν the mean intensity of radiation, at frequency ν.

As is customary in the stellar atmosphere theory, one expresses the total energy dissipated (and therefore radiated away) from the unit disk face area, $D(R) = \int D_{\mathrm{mech}}(z)dz$, through the *effective temperature*, T_{eff}, as $\sigma T_{\mathrm{eff}}^4 = D(r)$, where σ is the Stefan-Boltzmann constant. Assuming further a stationary, Keplerian disk, the effective temperature is given by

$$T_{\mathrm{eff}} = \left(\frac{3GM_*\dot{M}}{8\pi\sigma R^3} \left[1 - \left(\frac{R}{R_*} \right)^{1/2} \right] \right)^{1/4}$$

Summarizing the basic assumptions:

- disk is divided into a set of concentric rings, each behaving as an independent plane parallel radiating slab; no assumptions about optical thickness are made. One run of TLUSDISK calculates the vertical structure of one ring;

- hydrostatic equilibrium in the vertical z-direction;

- energy balance is considered as a balance between net radiation loss (calculated exactly, without invoking neither optically thin, nor optically thick [diffusion] approximations), and dissipated mechanical energy;

- dissipated energy is proportional to viscosity, which is given through Reynolds number;

- effect of illumination of disk by the central star are taken into account, using the formalism of Hubeny (1990b).

Disks around supermassive black holes

In this case, the above equations are modified because i) the presence of general relativistic effects (we adopt here a formalism of Riffert and Herold 1995); and ii) a possibility of using a different parametrization of viscosity. The equations are described in detail in Hubeny and Hubeny (1998). Here we describe some changes with respect to the above formalism.

The basics equations are modified as follows:

i) *Vertical hydrostatic equilibrium,*

$$\frac{dP}{dm} = g(z) \,, \tag{1}$$

where the depth-dependent vertical gravity acceleration is given by

$$g(z) = \frac{GM}{R^3} \frac{C}{B} \, z \,. \tag{2}$$

G is the gravitational constant, M is the black hole mass, and B and C (together with A and D used later) are the so-called relativistic corrections in the notation of Riffert and Harold (1995)..

ii) *Energy balance,*

$$\frac{9}{4} \frac{GM}{R^3} \left(\frac{A}{B}\right)^2 \rho \, w = 4\pi \int_0^\infty (\eta_\nu - \kappa_\nu J_\nu) d\nu \,. \tag{3}$$

The energy balance equation may be cast to different form if we do not express the radiation flux through the moment equation of the transfer equation, namely

$$\frac{dF_{\rm rad}}{dm} = -\frac{9}{4} \frac{GM}{R^3} \left(\frac{A}{B}\right)^2 w(m) \,. \tag{4}$$

The effective temperature is now given by

$$T_{\rm eff}^4 = \frac{3}{8\pi\sigma} \frac{GM\dot{M}}{R^3} \frac{D}{B} \,, \tag{5}$$

(iii) *Vertically-averaged viscosity*

The vertically-averaged kinematic viscosity is either given through the Reynolds number, as above; or through the effective α_0-parameter that relates the vertically-averaged stress to vertically-averaged pressure.

The vertically-averaged kinematic viscosity is given through α_0 as

$$\overline{w} = 2\dot{M}^2 \alpha_0 \sqrt{\frac{GM}{R^3}} \left(\frac{\sigma_e}{8\pi m_H c}\right)^2 \frac{D^2}{AC}, \tag{6}$$

where m_H is the mass of hydrogen atom, and σ_e the electron scattering (Thomson) cross-section. If one adopts the α-parametrization of viscosity, the total column mass is given by

$$m_0 = \frac{16\pi}{3} \left(\frac{m_H c}{\sigma_e}\right)^2 \sqrt{\frac{R^3}{GM}} \frac{1}{\dot{M}\alpha_0} \frac{BC}{AD}, \tag{7}$$

The relation between α_0 and Re is

$$Re = 2 \left(\frac{4\pi m_H c}{\sigma_e}\right)^2 \left(\frac{R}{\dot{M}}\right)^2 \frac{1}{\alpha_0} \frac{AC}{D^2}. \tag{8}$$

(iv) *Local viscosity*

The (depth-dependent) viscosity w is allowed to vary as a step-wise power law of the mass column density, viz.

$$w(m) = w_0 \left(m/m_0\right)^{\zeta_0}, \quad m > m_d, \tag{9}$$

$$w(m) = w_1 \left(m/m_0\right)^{\zeta_1}, \quad m < m_d, \tag{10}$$

where m_d is the division point. In other words, we allow for a different power-law exponent for inner and outer layers. This represents a generalization of an approach we used previously, based on a single power-law representation

We have thus four independent parameters: exponents ζ_0 and ζ_1, the division point, m_d, and the fraction, f, of energy dissipated in deep layers, $m > m_d$. The coefficients w_0 and w_1 are derived from the condition on the vertically averaged viscosity, $\int_0^{m_0} w(m)dm/m_0 = \overline{w}$, and $\int_{m_d}^{m_0} w(m)dm/m_0 = f\,\overline{w}$. We obtain

$$w_0 = \frac{f\,\overline{w}(\zeta_0 + 1)}{1 - (m_d/m_0)^{\zeta_0+1}}, \tag{11}$$

$$w_1 = \frac{(1-f)\,\overline{w}(\zeta_1 + 1)}{(m_d/m_0)^{\zeta_1+1}}. \tag{12}$$

Generally, $w(m)$ does not have to be continuous at the division point m_d. If we require the continuity, then f and m_d are no longer two independent parameters; instead, they are related through

$$\frac{m_d}{m_0} = \left(1 + \frac{\zeta_0 + 1}{\zeta_1 + 1}\frac{f}{1 - f}\right)^{-\frac{1}{\zeta_0+1}}. \tag{13}$$

Typically, the deep-layer power law exponent ζ_0 is set to 0 (constant viscosity), while the "surface" power law exponent ζ_1 is usually set to a value larger than zero.

In TLUSTY, parameter ζ_0 is set by the optional parameter ZETA0; parameter ζ_1 is set by the optional parameter ZETA1; parameter f is set by the optional parameter FRACTV; and the division point m_d is set by the optional parameter DMVISC;

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