TLUSTY User's Guide III: Operational Manual

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Abstract

This paper presents a detailed operational manual for TLUSTY. It provides a guide for understanding the essential features and the basic modes of operation of the program. To help the user, it is divided into two parts. The first part describes the most important input parameters and available numerical options. The second part covers additional details and a comprehensive description of all physical and numerical options, and a description of all input parameters, many of which needed only in special cases.

Contents

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Part I

1 Introduction

The following document is a comprehensive guide to the operation of the program. It describes in detail the structure of the required input files and resulting output files, and explains the meaning of the individual input parameters. To help the user, the explanations are supplemented by a number of actual examples of input files for model atmospheres of various stellar types that may be used as templates for a construction of similar models.

The program allows for a large number of options, controlling both the physical as well as numerical setup of the calculations. While some options are very important or even critical for the numerical performance of the code and the quality of the model, there are many options and parameters that are important only in special cases. This document is therefore divided into two parts. The first part deals with the basic numerical implementation and provides a guide for understanding the essential features and a basic operation of the program. Additional details, a comprehensive description of all physical and numerical options, and a description of all input parameters, most of which needed only in special cases, are described in Part II.

2 Compiling and linking

2.1 Compilation

The program is distributed as several files. The largest is `tlusty[nnn].f` where `nnn` represents the current version number. In the following text, we take 205 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 `tlusty205.f` file, and, under UNIX/LINUX, 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 with any new version of TLUSTY. In the standard distribution, described in Paper I, § 3.1, the source file as well as the INCLUDE files are indeed located in the same directory.

The compilation is done as follows:

• Under Mac OSX, or modern versions of Linux

```
gfortran -fno-automatic [-O3] [-o tlusty] tlusty205.f
```

where the option `"-fno-automatic"` indicates the static allocation of memory, which is a mandatory option. The level-3 optimization (`"-O3"`) should be switched on since it improves the performance of the code considerably. Reaming the executable as specified by `"-o tlusty"` allows the user to use script file `RTlusty` to conveniently run TLUSTY.

• Under older versions of LINUX

```
f77 -fno-automatic [-O3] [-o tlusty] tlusty205.f
```

• Under generic UNIX

```
f77 [-O4] [-static] [-Nl100] [-o tlusty] tlusty205.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 equivalent to `"‘-fno-automatic"`, is needed for some variants of UNIX. It is a default in most implementations. Similarly, the optimization (the option `"-O4"`) is a default on most workstations. If not, the optimization should be switched on since it improves the performance of the code considerably.

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

```
pgf77  [-Bstatic] [-fastsse] [-o tlusty] tlusty205.f
```

2.2 Reducing the size of the executable file

The strategy adopted in early days of the development of TLUSTY, before FORTRAN90 was introduced, was to code the maximum dimensions of the important arrays that determine the overall memory consumption of the code in a few special files, communicated through the `INCLUDE` statements. This way it became possible to easily change array dimensions, and thus the memory needed, by simple changing a few lines in the INCLUDE files. Although the memory consumption is no longer such a critical issue as it used to be in the past, it may still be sometimes necessary to change the overall memory requirements. For instance, one has to be careful not to exceed 2 GB of core memory, a typical value of a medium-class Mac or a LINUX box, when computing NLTE metal line-blanketed models.

The basic parameters defining array dimensions appear in the INCLUDE file `BASICS.FOR`. The first `PARAMETER` statement there contains the most important parameters; which we list below. Their exact meaning is explained through this paper.

MATOM	maximum number of atomic species
MION	maximum number of explicit ions
MLEVEL	maximum number of explicit levels
MLVEXP	maximum number of explicitly linearized levels
MTRANS	maximum number of all transitions
MDEPTH	maximum number of depth points
MFREQ	maximum number of frequencies
MFREQP	maximum dimension of working arrays for setting superlines
MFREQC	maximum number of frequencies in continua
MFREX	maximum number of linearized frequencies
MFREQL	maximum number of frequencies per line
MTOT	maximum number of linearized parameters (ie. maximum dimension of vector ψ)
MMU	maximum number of angle points

There are also secondary parameters; their values are rarely changed. Here is their list:

MBF	maximum number of bound-free transitions
MCROSS	maximum number of photoionization cross sections plus related quantities
MFIT	maximum number of fit points for the input of bound-free cross sections
MITJ	maximum number of lines contributing to the opacity at a given frequency
MMCDW	maximum number of levels with pseudocontinuum
MMER	maximum number of "merged" levels
MZZ	maximum charge of an ion treated with occupation probabilities
MVOIGT	maximum number of lines with Voigt profiles
MSMX	size of largest matrix kept in memory in SOLVE

The above parameters are universal. There are also other parameters which specify dimensions of arrays which are being used only under special circumstances (including using the opacity tables, Compton scattering; tri-diagonal approximate operator, etc.), which are set to 1 for the bulk of applications. These are the following:

MFRTAB	maximum number of frequencies in the opacity table; if opacity table is not used, =1
MTABT	maximum number of temperatures in the opacity table
MTABR	maximum number of densities in the opacity table
MFREQ1	set to MFREQ in case of Compton scattering or DFE transfer solver; otherwise =1
MDEPTC	set to MDEPTH in case of Compton scattering; otherwise =1
MMUC	maximum number of angle points for Compton scattering

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 the 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 a superline coss section (obsolete)
MHOD maximum number of merged-levels cross sections
MDODF maximum number of depth points for storing the superline cross sections
MKULEV maximum number of internal energy levels for an ion treated by means of opacity sampling; if opacity sampling is not used, it should be set to 1
MLINE maximum number of internal lines for an ion treated by means of opacity sampling; if opacity sampling is not used, it should be set to 1
MCFE maximum total number of internal lines for all ions treated by means of opacity sampling; if opacity sampling is not used, it should be set to 1

The program checks whether the current values are less than or equal to the corresponding maximum dimension, and stops if there is a conflict. The program then issues a brief message (on the standard output and on the special performance and error message file), showing the corresponding current and maximum values. The program should then be recompiled with the corresponding parameter appropriately modified in the 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 exception from this rule is `MDEPTH` and the 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 the INCLUDE files `BASICS.FOR` and `ODFPAR.FOR`). 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.

We stress that the standard distribution of TLUSTY, as specified in Paper I, § 3.1 contains the INCLUDE files `BASICS.FOR` and `ODFPAR.FOR` that specify the basic array dimensions in such a way that one can run all the test cases described in Chapter 6, including a metal line-blanketed model atmosphere of a B star

(§ 6.3). In other words, the dimensions are relatively large, and the executable takes about 1.7 GB of memory. If the user does not have a computer with 2 GB of core memory or more, then he/she have to modify the files accordingly, for instance by decreasing the values of the critical parameters in `ODFPAR.FOR` to 1, which would allow to run all tests cases in Chapter 6 except the one for a B star.

2.3 Program PRETLUS

Setting the maximum dimensions of arrays may be a delicate task because in many instances the actual dimensions depend on input data in a rather non-trivial manner. In order to assist the user in setting the dimensions of arrays, and consequently to reduce the size of the executable file, we have developed a utility program PRETLUS, which is distributed along with the the main TLUSTY program.

Program PRETLUS is easy to run. It accepts exactly the same input as TLUSTY, and it essentially performs the initialization part of TLUSTY without any actual calculations, and outputs the list of actual dimensions of all important arrays. The user has too check files `BASIC.FOR` and `ODFPAR.FOR` to make sure that the values of the dimension parameters given there are equal or larger than the actual values listed in the standard output from program PRETLUS. An example of the output produced by PRETLUS is given in § 6.3.

3 General scheme of the input

3.1 Overview

The essential feature of the input data format is that there is only a very short standard input file, which specifies (i) the very basic parameters ($T_{\rm eff}, \log g$) for which no reasonable default values can be specified; (ii) the name of the file where the optional, or keyword, parameters are set up; and (iii) the names of files where the atomic data for the individual ions are stored. Keyword 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 case. Keyword parameters also allow the user to choose among several alternative numerical schemes, or to cope with convergence problems. The most important ones are described in Chap. 7, the remaining ones in Chaps. 12 and 13, and the full list of keyword parameters together with their default values is presented in Chap. 16.

Here is a list of input files.

- `fort.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, a stellar atmosphere model is to be computed. Otherwise, a disk vertical structure is computed.

- Standard input file (unit 5) — Main control data. It is 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 are explained in Chap. 4.

- File that specifies non-default values of the keyword parameters. Its name is specified in the standard input file.

- `fort.8` — A starting model atmosphere (if the calculation does not start from the scratch, that is, with an LTE-gray model) - see Chap. 8.

These are universal input files that need to be supplied for any mode of operation.

In the standard mode, where the opacities are computed on the fly, and where one introduces the concept of explicit ions and levels (which is mandatory for NLTE models), there is an important set of input files, namely

- Files containing atomic data for the individual ions. These files are described in detail in Chap. 11. A collection of such files is a part of the standard distribution. It is also available on the TLUSTY website.

Further, depending on the mode of application, which is set up by appropriate keyword parameters, there may be additional input files, which are also a part of the standard distribution of TLUSTY, namely:

- `lemke.dat` or `tremblay.dat` – special hydrogen line broadening tables – see also § 12.1.1

- Special tables for hydrogen quasi-molecular data – see also § 12.1.2

- `tsuji.molec` – a table with necessary parameters for the molecular state equation – see also § 6.4, § 7.4.1 and § 7.10.3

- `irwin.dat` – a table of Irwin partition functions – see also § 12.7

In the case where some or all opacities are supplied from the pre-calculated opacity tables, one needs the following input files:

- `absopac.dat` – opacity table, required if IOPTAB=−1 – see also § 6.4 and § 13.1

- Rayleigh scattering opacity table; if required – see also § 12.2.1

- State equation tables, if required. Notice that when using the full opacity table option, one can still solve the equation of state and compute the thermodynamic parameters needed for treating convection on the fly, so these tables may not be required.

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 with `*` or `!` as comment. The structure of these files is explained in detail below.

3.2 What needs to be specified?

There are two types of input parameters; the true *physical quantities* (such as the effective temperature, $T_{\rm eff}$), 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 a 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 the user in such a way that important parameters have to be set up in the standard input file, while other, either less important, or newly introduced parameters, assume their default values unless the user specifically requires to change them. This is done through the keyword parameters file.

As the code evolves, it is often necessary to introduce new input parameters. These are set through the keyword parameter file, even if they may sometimes be quite important. A practical reason for setting newly introduced parameters in the keyword parameter file instead of the standard input is that there is a large library of standard input files for various models, and it would be cumbersome to be forced to change them whenever a new important input parameter is introduced.

We list the essential categories of the input parameters below.

- Basic model parameters.
  These are $T_{\rm eff}$ 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 § 4.1.

- Setting LTE or NLTE.
  This is done in the standard input, see § 4.1.

- Chemical composition and the choice of explicit species.
  We recall that 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 the kinetic equilibrium equations. 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 that is calculated on the fly, but is allowed to contribute to the total number of particles and to the total charge; the latter is evaluated assuming LTE ionization balance, i.e., by solving a set of Saha equations. The choice of explicit and implicit atoms, together with their abundances, is given in the standard input – see § 4.2.

- Choice of explicit ions.
  Again, the choice has to be made judiciously, as it significantly influences

the overall quality of a model. The choice is also given in the standard input – see § 4.3. Notice that if the full opacity table option is adopted, there are no explicit ions defined.

- Atomic data for explicit ions.
  This is an important, and sometimes decisive, ingredient of good NLTE models. The standard input file specifies the filenames of the individual atomic data for each explicit ion; the atomic/ionic data files are separate. This enables us to store these individual 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 § 15.1). Again, in the case of using full opacity tables, there is no need to have these files.

- Auxiliary physical parameters.
  Here we have for instance convection parameters, microturbulent velocity, possible external irradiation intensity, etc. As explained in the next chapters, 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 keyword parameters file, discussed in detail in Chap. 7.

- 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 keyword parameters. The actual values of the individual column masses (which is the default depth coordinate) are either given in the input model, or are constructed in the starting LTE-grey model atmosphere. The corresponding parameters are also set up by the keyword parameters - see § 7.5. 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 § 4.1, and through several optional keyword parameters – see § 7.4.2 and § 7.7.

- Numerical options
  There is a large number of flags for controlling many numerical aspects, usually communicated as keyword parameters – see Chaps. 7 and 15. As mentioned above, the atomic data files also contain some flags of this category. If the model computation proceeds well without any special keyword

parameters file, that is if the default values of keyword parameters provide a satisfactory numerical strategy, the user does not have to set up this file. However, in a majority of cases one needs to set up some optional keyword parameters, so one is recommended to obtain at least a rudimentary knowledge from Chap. 7; more dedicated users are encouraged to study also Chaps. 12 and 13 in detail. A practical advice how to use various options for troubleshooting is briefly summarized in Chap. 15.

4 Standard input file

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

4.1 First block – Basic Parameters

This block contains only four lines of input.

First 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 three 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 $T_{\rm eff}$, Q, and m_0.

Specifically, if XMSTAR > 0, then the subsequent three parameters are:

XMDOT – mass accretion rate. It can be expressed in g/s, or in $M_\odot$/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 disk, 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 Kerr black hole with maximum stable rotation).

RELDST – relative distance of a given annulus with respect to the stellar radius (classical case), or the 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, $Q = \Omega_{\rm K}^2$, where $\Omega_{\rm K}$ is the Keplerian velocity, $\Omega_{\rm K} = (GM/R^3)^{1/2}$.

DMTOT – column mass at the midplane (=1/2 of the total column mass) [g]

Second 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-gray 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 (`fort.8`) input.

Third line:

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

Fourth line:

NFREAD – an indicator of the number of frequency points and their setup:
> 0 – the program sets up the *continuum* frequency points. We stress that the frequency points in the lines are set up separately based on the input data contained in the input atomic data files. The details of setup are governed by several keyword parameters (FRCMAX, FRCMIN, CFRMAX, NFTAIL, and DFTAIL – see Sect.7.4.2). In the default case, the program sets two frequencies near discontinuities 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 keyword parameters FRCMAX and FRCMIN, respectively; the number of points in the high-frequency tail are specified by the keyword parameters NFTAIL and DFTAIL. (i.e. they may be changed by a corresponding specification in the input file FINSTD).
< 0 – the frequency points are set up logarithmically equidistant between FRCMIN and FRCMAX, with the total number abs(NFREQ).

4.2 Second block – Selection of, and basic data for, chemical species

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.). TLUSTY can potentially treat elements with atomic number 1 – 99, but in practice only a smaller number of elements (typically 30) are taken into account. Another concern is that the values of the partition functions for species with atomic number higher than 30 are hardwired only for the first two ionization stages, so when treating higher ions of such species the user has to supply the corresponding expressions or tables.

The individual input parameters have the following meaning:

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).
$= 0$ – no explicit atoms are selected. This option only makes sense in the case of using complete pre-calculated opacity and state equation tables (set by the keyword parameter IOPTAB $= -2$).

MODE – a specification of the mode of treatment of the given species:
$= 0$ – the element is not considered at all;
$= 1$ – he element is treated *implicitly*. In this case, the species does not

contribute to the opacity; but it is allowed to contribute to the total number of particles and to the total charge; the latter is evaluated assuming LTE ionization balance, i.e., by solving a set of Saha equations.
= 2 – the element is treated *explicitly*, i.e., selected energy levels of of the selected ionization states are considered explicitly; i.e., their populations are determined by solving the corresponding kinetic equilibrium equations.

ABN – a specification of the abundance of the given species:
= 0 – the solar abundance is assumed (Grevesse & Sauval 1998) – see Paper II, Table 1;
< 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 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 means of the optional parameter IATREF (see Sect. 7.4.4)
$> 10^6$ – non-homogeneous (depth-dependent) abundance is assumed. In this case, the immediately following *ND* lines should be added that contain the individual values of the abundance (relative to hydrogen by number), for all depth points $d = 1, \ldots, ND$.

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 – see Paper II, § 2.7
> 0 – the partition functions evaluated from the Opacity Project ionization fraction tables.
< 0 – non-standard evaluation by a user-supplied formula to be implemented in subroutine PFSPEC. For details, refer to § 14.4.

4.3 Third block – Explicit ions

For each ion, including the highest ionization degree of a given species, there must be one input record for each of then relevant ionization stages 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 explicit ions input block.

ILVLIN – an indicator of changing the treatment of a whole group of bound-bound transitions, regardless of the input communicated by the atomic data file - see below. ILVLIN has the meaning that all lines with the relative index of the lower level smaller than ILVLIN are considered in detailed radiative balance and their opacity is neglected. 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 atomic input files for LTE, NLTE/C (NLTE with continua only), and NLTE/L (NLTE with lines) models – see below.

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 applications), or to provide necessary filenames for treating ions for which the superlevel and superline formalism is used (typically the iron-peak elements).
$= 0$ – no change of non-standard parameters is required;
> 0 – additional record with "non-standard" parameters. This is a more or less outdated option; for completeness see § 11.6;
< 0 – additional record(s) with filenames for evaluating cross sections for superlines– see below. Moreover, when superlines are treated in the Opacity Sampling option, the actual numerical value of NONSTD defines the formation of superlines, namely:
$= -1$ – all internal lines contribute to an appropriate superline;
$= -2$ – all internal lines except autoionizing lines (with upper levels above the ionization potential) contribute; autoionizing lines are neglected;
< -2 – only lines between observed levels (internal levels with measured energies) are considered.

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 Chap. 11.

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`.

If the parameter NONSTD of the standard input (see above) is coded as negative, the program reads an additional record with the following four parameters:

INODF1, INODF2 – unit numbers for pre-computed data for superline cross sections treated through Opacity Distribution Function (ODF). This is now an outdated option, these two numbers should bet set to zero, INODF1 = INODF2 = 0.

FIODF1, FIODF2 – filenames for evaluating superline cross sections:
– in the standard case of the Opacity Sampling (OS), the first file is the Kurucz level data file (e.g., `gf2601.gam`, for Fe II), and the second file is the line data file (`gf2601.lin`).
– in the (outdated) case of ODF treatment of lines, the filenames of the corresponding ODF input.

FIBFCS – the name of the file containing the photoionization cross sections for the individual superlevels. The parameters IFANCY (see Sect. 11.2) has to be set to a value between 50 and 99 to switch on reading cross sections from a previously created file.

5 General strategy of model construction

As explained in Paper II, § 3.1 – 3.3, any variant of the linearization scheme that is used for constructing model atmospheres is quite sensitive to a quality of the initial estimate. This feature dictates the strategy of constructing models, which often consists in a series of consecutive steps. We shall describe several possible approaches below.

5.1 LTE models

Constructing an LTE model is usually relatively straightforward. The strategy depends on whether an LTE model to be computed is used as a starting solution for a subsequent NLTE model, or whether it is the final result on its own right. In the former case, the model can be quite simple, for instance without taking into account lines. In the latter case, one aims at achieving a much higher degree of complexity of the model, which usually requires more refined modeling techniques.

As mentioned earlier, an attractive option to construct an LTE model is using a pre-calculated opacity table. This can in principle be done at any temperature range, but at the moment our opacity table only covers temperatures between 4000 and 10,000 K, so it can be used only for G and K star atmospheres. We plan to extend the opacity table to lower temperatures (say, down to 100 K). An extension to higher temperatures is possible as well, and in fact is relatively easy,

but it would not have much practical value because LTE model atmospheres are not accurate enough for higher temperatures (say, for effective temperatures above 15,000 K).

There are several possibilities to construct an LTE model atmosphere:

(i) The standard way is to start from the scratch; that is, first to construct an initial LTE-gray model, and immediately continue to converge the desired LTE model. As shown in the previous chapter, this is done in one step. Some examples are shown in § 6.2 (a simple H-He model), and § 6.4 (a complex line-blanketed model, computed using an opacity table).

(ii) One can use an existing LTE model, either constructed earlier by TLUSTY, or taking a Kurucz model atmosphere, as a starting mode atmosphere, and converge the desired LTE model from it. Obviously, the basic input parameters, $T_{\rm eft}$ and $\log g$ for the input model must not be very different from $T_{\rm eff}$ and $\log g$ of the model to be constructed. A conservative estimate is to change $T_{\rm eff}$ by no more than 5-10%, and $\log g$ by no more than 0.2 dex. Otherwise, the model may still converge, but could easily take more computer time than when starting from the scratch.

(iii) When constructing a line-blanketed model without using an opacity table, one has to proceed in at least two steps. The first step consists of computing a simple model starting from the scratch (typically without any lines), and the next step includes all the lines. The reason for this procedure is that the adopted treatment of metal line blanketing needs an input starting model in order to construct the appropriate cross sections for superlines.

(iv) For complex or difficult models, it is possible to construct the desired model by a sequence of intermediate models. Typically, one first converges a model with a few or no lines considered explicitly, and then one adds lines. This approach is analogous to an often used strategy of constructing NLTE models, which will be described below.

5.2 NLTE models

A usual strategy, adopted already in the pioneering study of Auer & Mihalas (1969) is to proceed in three steps:

LTE $\rightarrow$ NLTE/C $\rightarrow$ NLTE/L,

where NLTE/C represents a NLTE model with continua only; i.e., without lines. In other words, all lines are taken in detailed radiative balance (their radiative rates are set to 0), and their opacity is neglected. NLTE/L denotes a NLTE with lines. We stress again that the LTE model used for this purposes does not have to be a sophisticated LTE model; typically an LTE without lines is sufficient.

The reason for adopting this procedure is the following: We know that with increasing depth in the atmosphere departures from LTE generally decrease, so deep enough the state of the atmosphere is well described by an LTE model. The continua (bound-free atomic transitions) are typically less opaque than the bound-bound transitions (lines), so they are formed deeper in the atmosphere.

Therefore, including continua only in an NLTE model yields an essentially exact atmospheric structure in deep, continuum-forming, layers. Including lines in the final step then corrects the structure closer to the surface. By this strategy, one gradually improves the structure from deep layers to the surface, which is exactly how the energy in the atmosphere typically flows. (This also hints why a construction of an atmospheric model with a strong external irradiation may be numerically difficult).

The above reasoning also explains why it is sometimes advantageous to split the third step into several parts:

$$\text{NLTE/L1} \rightarrow \text{NLTE/L2} \rightarrow \ldots \rightarrow \text{NLTE/L},$$

where the individual steps consist of adding more and more lines. We stress that in some cases this is not necessary, and a final NLTE/L model can be constructed in one step. But often this is a good way to proceed. The simplest possibility, always worth trying in case of convergence problems with an NLTE/L model, is first to set a detailed balance in all the resonance lines (those with lower levels being the ground states of the corresponding ions), and then switch them on, perhaps in several steps starting with weaker resonance lines (those of less abundant ions), and ending with the strongest ones. The reason for this strategy is exactly the same as that put forward for the general strategy of improving the atmospheric structure going from deep to upper layers.

In some cases, in particular for models where departures from LTE are not crucial, say for late B stars and cooler, and also for hot white dwarfs that contain significant amounts of metals, the following procedure often proves advantageous:

$$\text{LTE/C} \rightarrow \text{LTE/L} \rightarrow \text{NLTE/L},$$

that is, constructing first a simple LTE model, than a fully blanketed LTE model (denoted LTE/L), and from it to proceed directly to fully blanketed NLTE/L model with all lines. This strategy reflects the physical fact that when NLTE effects are week, the most important mechanism for determining the atmospheric structure is the metal line blanketing.

5.3 Setting a detailed balance in lines

One may set up a detailed radiative balance in a line, and therefore exclude the corresponding transition rate from the kinetic 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 § 11.3). This is the most flexible way, but also the 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 § 4.3) for a given atom/ion, which is set in the standard input. The meaning of ILVLIN is that all lines originating at level with index lower than ILVLIN are set 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.

(iii) The third way to set lines to detailed balance is based on their frequency. This is driven by keyword parameters FRLMAX and FRLMIN (see § 7.4.2), which put 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 the laser effect in lines, which may lead to numerical problems.

6 Examples of standard input; test cases

6.1 General remarks about running TLUSTY

As already mentioned in Paper I, § 4.4, while the names of the TLUSTY input and output files can be arbitrary, it is advantageous to use the following convention: Any name of an input or output file is composed of a *core name* that may label the basic physical parameters of a model, with an extension identifying the unit number. For example, let us take a H-He model for $T_{\rm eff} = 35,000$ K and $\log g = 4$, in LTE. Let the core name be `hhe35lt`, so the standard input file is then `hhe35lt.5`. This example is considered below in § 6.2.

As is shown in Paper I, § 4.4, TLUSTY can be run as

```
tlusty.exe < [std.input_file] > [std. output_file]
```

but in this case the executable file `tlusty.exe` has to be present in (or liked to) the current directory, and also the necessary atomic data have to be copied or linked to the files specified by the standard input.

An easier and in fact a safer way is to use the shell script `RTlusty`, which is also a part of the standard distribution of TLUSTY. It is called with one or two parameters,

```
RTlusty   model_core_name   [core_name_of_starting_model]
```

The second parameter does not have to be present if the model is calculated from scratch.

We stress that the script `RTlusty` is designed to run a model in any directory provided that the two following requirements are fulfilled:

- One sets the environment variable `TLUSTY` that specifies the main TLUSTY directory. For instance, using the tar files downloaded from the Arizona site[1], and assuming that the tar file is extracted in the home directory, so the main TLUSTY directory is generated as `~/tlusty205`, one sets

  ```
  setenv TLUSTY ~/tlusty205
  ```

[1] http://aegis.as.arizona.edu/~hubeny/pub/tlusty205.tar.gz

- The universal directory containing atomic data is a subdirectory of the main TLUSTY directory, that is $TLUSTY/data

The script RTlusty has the following content:

```
#!/bin/bash
#
#       shell script to run tlusty
#
#       print syntax if no parameters specified
#
   if [ $# -lt 1 ]
   then
     echo Usage:
     echo RTlusty  model core name  [core name of starting model]
     exit
   fi
#
# check that the starting model exists
#
   if [ $# -eq 2 ]
   then
     if [ -e $2.7 ] ; then
         echo STARTING MODEL: $2.7;
      else
         echo FILE $2.7 does not exist, therefore quitting ;
         exit;
     fi
#
     rm -f fort.8
     cp $2.7 fort.8
   fi
#
#    link the "data" directory
#
   ln -s -f $TLUSTY/data data
#
#    run tlusty
#
   MOD=$1
   $TLUSTY/tlusty/tlusty.exe  < $MOD.5 > $MOD.6
#
#    save important output files
#
   cp fort.7 $MOD.7
   cp fort.9 $MOD.9
```

```
   cp fort.69 $MOD.69
   cp fort.13 $MOD.13
#
   echo "COMPUTED MODEL  $MOD  FINISHED!"
   date
#
```

Let us take an example from the next section, § 6.2, with the name of the input file being `hhe35lt.5`. Then the code can be either as

```
tlusty.exe < hhe35lt.5 > hhe35lt.6
```

where the standard output is redirected to a file `hhe25lt.6` for further inspection; or one can use the script `RTlusty` and to run the test as (this time in the background)

```
RTlusty hhe35lt &
```

which runs the code and stores not only the standard output (unit 6) but also other important output files, all with the same core name, and with the suffix that corresponds to the unit number. They are explained in more detail in § 9.1. Briefly, `hhe35lt.7` contains a condensed model atmosphere, `hhe35lt.9` the convergence log, `hhe35lt.13` the emergent flux, and `hhe35lt.69` the timing log. There are more output files; if they are intended to be kept for future use, they should be renamed, perhaps with the same core name.

After a completed run, it is very important to inspect the convergence log to make sure that all the relative changes of the components of the state vector are sufficiently small. The standard distribution of TLUSTY also contains an IDL program `pconv.pro` which plots the contents of the convergence log. The program needs three output files, units 7, 9, and 69, and assumes that the file names are constructed using the above convention, that is the core names are the same. The program It is called as

```
pconv,'hhe35lt'
```

It can be called also as

```
pconv
```

in which case the files are supposed to have generic names `fort.*`. Several examples of plots generated by `pconv` are presented throughout this chapter.

It is also important to inspect the last table of the standard output; in the present case `hhe35lt.6`, which summarizes the computed model atmosphere. The last four columns show the computed total flux (radiative plus, if applicable, convective), and the ratios of the radiative, convective, and computed total fluxes with respect to the theoretical total flux, $\sigma T_{\rm eff}^4$, respectively. Therefore, the values of the last column should be very close to unity (up to at most 1% departures from it); otherwise the model cannot be viewed as sufficiently accurate, even if the convergence log may show that the model is formally converged.

6.2 Simple H-He model atmosphere from scratch

A simple LTE model atmosphere with $T_{\rm eff} = 35{,}000$ K, $\log g = 4$, composed of H and He (treated as explicit), and C, N, O (implicit; taken only for particle and charge conservation), is constructed by TLUSTY by setting the standard input as follows – file `hhe35lt.5`:

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

As mentioned before, one has to make a link from a standard "data" directory to `./data` refereed to in the input file. When using the `RTlusty` script, this is done automatically.

The files `h1.dat, he1.dat, he2.dat` contain necessary atomic data for H I, He I, and He II, respectively. Structure of these, as well as other atomic data

files, is explained in detail in Chap. 11. Here we assume that the model 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, because these ions have no internal structure. Since the `ILVLIN` parameters are set to 100, higher than the number of levels, all lines are set to detailed radiative balance, and their opacity is neglected. This model, and its convergence properties were already shown in Paper 1, § 3.4.

The corresponding NLTE/C model is constructed with virtually the same standard input; the only change is replacing the second record by:

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

The file is stored as `hhe35nc.5`, The model is run, using the script]`RTlusty` as

```
RTlusty hhe35nc hhe35lt
```

where the second parameter, `hhe35lt`, stipulates that the starting model is taken as the result of the previous run, `hhe35lt.7`.

The frequency points in both previous models are set up with the default values of the highest frequency, (such as $\nu_{\rm max} = 10^{11} T_{\rm eff}$ – see § 7.4.2), the lowest frequency $\nu_{\rm min} = 10^{12}$. The number of frequency points is approximately 50+2×(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 128 because unnecessary frequency points for the He II edges that coincide with H edges are removed.

The final NLTE/L model (NLTE with lines), considering all lines of H and He explicitly, is calculated by modifying the fourth block of the standard input file (stored as `hhe35nl.5`) as follows:

```
*
*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    14      0      0      0    'He 1' './data/he1.dat'
   2     1    14      0      0      0    'He 2' './data/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 with the default values of the highest frequency, (such as $\nu_{\rm max} = 10^{11} T_{\rm eff}$ – see the next Section), the lowest frequency $\nu_{\rm min} = 10^{12}$. The number of frequency points is approximately 50+2×(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

128 because unnecessary frequency points for the He II edges that coincide with H edges are removed.

The run is generated analogously as before,

```
RTlusty hhe35nl hhe35nc
```

The convergence log, displayed using the IDL program `pconv`, is shown in in Fig. 1. As in the analogous Fig. 1 of Paper I, there are six panels on the figure, the upper three display the relative changes of temperature (which is usually the most important component of the state vector), while the lower three panels show the maximum relative change of all components of the state vector. The leftmost panels show the relative change as a function of column mass in the absolute scale, and the middle panels the same in the logarithmic scale. We display both, because the linear scale shows the sign of the relative changes but does not properly show those that are small. These are in turn clearly seen on the logarithmic scale. The rightmost panels show the maximum relative change over all depth points. This is an indicator of the global convergence of the model. Ideally, the relative changes should gradually decrease, which was clearly the case here. The convergence is slower than for the LTE corresponding model, but still stable. The effects of the Ng acceleration are seen in the 7th iteration, and then after each 4 iteration steps. The figure also contains a header that displays the core name and the total execution time. In the present case, it is 23 s, longer than for the LTE model presented in Paper 1, which was less than 1 s. This, and all other calculations reported below, were done on MacBook Pro, with 2.2.GHz Intel Core i7.

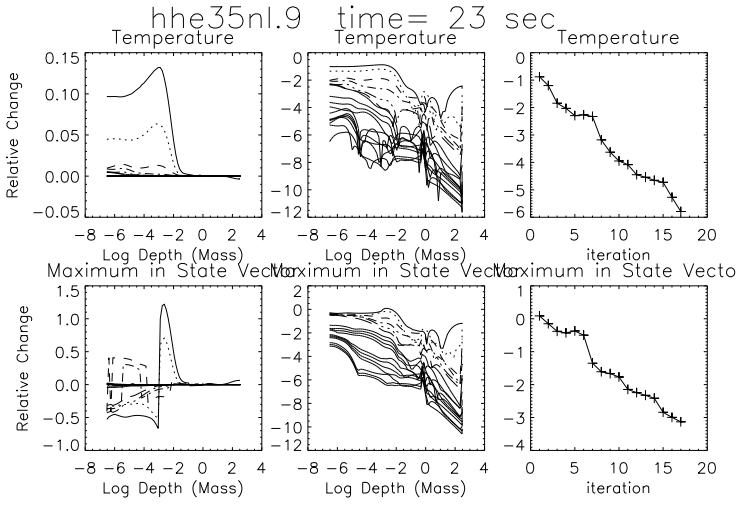

Figure 1: Convergence log for the NLTE/L H-He model.

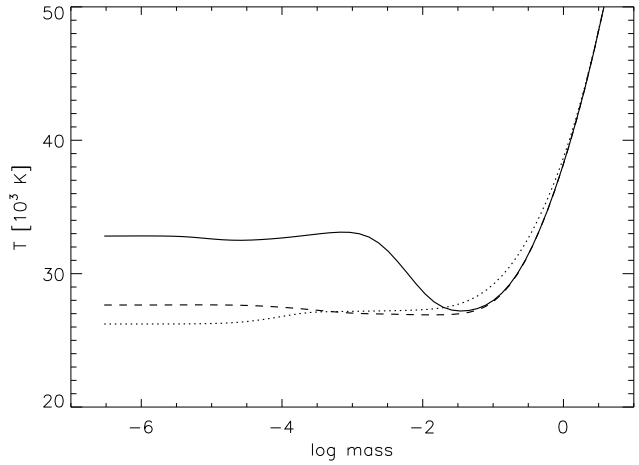

Figure 2: Temperature as a function of column mass for the three H-He modes: NLTE/L (full line), NLTE/C (dashed line), and LTE (dotted line).

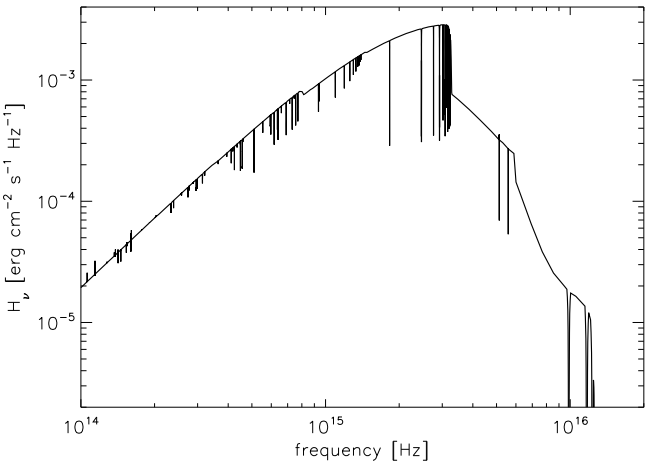

Figure 3: Emergent flux for the H-He NLTE/L model.

Figure 2 displays the temperature structure for all the three models. The most interesting feature is a temperature rise at the surface, first discovered by Auer & Mihalas (1969), and explained as an indirect effect of the Lyman α line on the heating rate in the Lyman continuum. The plot also shows that the temperature structure for both NLTE models approaches that of the LTE model deep in the atmospheres (around $\log m \approx 0.5$ in the present case), and that the temperature structure for the NLTE/C and NLTE/L models start to differ around $\log m \approx -1$ where lines become transparent.

Figure 3 shows the emergent flux (better speaking, H_ν) as a function of frequency, which is given by the first two columns of the file `hhe35nl.13`. We stress that this is the flux produced directly by TLUSTY, and which is only a schematic representation of the exact emergent flux because lines of only H and He are taken into account. One can construct a detailed spectrum, including all lines, using the associated program SYNSPEC. This was shown in Paper I, § 4.7.

6.3 NLTE line-blanketed B star model atmosphere

A complex example is provided for a NLTE line-blanketed B star model atmosphere, with $T_{\rm eff}$ = 20,000 K, $\log g = 4$, with a solar metallicity. This example corresponds to the data used for calculating the BSTAR2006 grid (Lanz & Hubeny 2007), file `BGA20000g400v2.5`, which is called here `BGA20000g400v2a.5` to stress that one will construct a different model.

```
20000. 4.0
 F  F              ! LTE,  LTGRAY
 'nst'             ! keyword parameters filename
*
* 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.      0  ! C
    2   0.      0  ! N
    2   0.      0  ! O
    1   0.      0
    2   0.      0  ! Ne
```

```
    1   0.      0
    2   0.      0  ! Mg
    2   0.      0  ! Al
    2   0.      0  ! Si
    1   0.      0
    2   0.      0  ! S
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    2   0.      0  ! Fe
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      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/he1.dat'
   2    1    20      0      0      0    'He 2' 'data/he2.dat'
   2    2     1      1      0      0    'He 3' ' '
   6    0    40      0      0      0    ' C 1' 'data/c1.dat'
   6    1    22      0      0      0    ' C 2' 'data/c2.dat'
   6    2    46      0      0      0    ' C 3' 'data/c3_34+12lev.dat'
   6    3    25      0      0      0    ' C 4' 'data/c4.dat'
   6    4     1      1      0      0    ' C 5' ' '
   7    0    34      0      0      0    ' N 1' 'data/n1.dat'
   7    1    42      0      0      0    ' N 2' 'data/n2_32+10lev.dat'
   7    2    32      0      0      0    ' N 3' 'data/n3.dat'
   7    3    48      0      0      0    ' N 4' 'data/n4_34+14lev.dat'
   7    4    16      0      0      0    ' N 5' 'data/n5.dat'
   7    5     1      1      0      0    ' N 6' ' '
   8    0    33      0      0      0    ' O 1' 'data/o1_23+10lev.dat'
   8    1    48      0      0      0    ' O 2' 'data/o2_36+12lev.dat'
   8    2    41      0      0      0    ' O 3' 'data/o3_28+13lev.dat'
```

```
  8    3    39     0     0     0    ' O 4' 'data/o4.dat'
  8    4     6     0     0     0    ' O 5' 'data/o5.dat'
  8    5     1     1     0     0    ' O 6' ' '
 10    0    35     0     0     0    'Ne 1' 'data/ne1_23+12lev.dat'
 10    1    32     0     0     0    'Ne 2' 'data/ne2_23+9lev.dat'
 10    2    34     0     0     0    'Ne 3' 'data/ne3_22+12lev.dat'
 10    3    12     0     0     0    'Ne 4' 'data/ne4.dat'
 10    4     1     1     0     0    'Ne 5' ' '
 12    1    25     0     0     0    'Mg 2' 'data/mg2.dat'
 12    2     1     1     0     0    'Mg 3' ' '
 13    1    29     0     0     0    'Al 2' 'data/al2_20+9lev.dat'
 13    2    23     0     0     0    'Al 3' 'data/al3_19+4lev.dat'
 13    3     1     1     0     0    'Al 4' ' '
 14    1    40     0     0     0    'Si 2' 'data/si2_36+4lev.dat'
 14    2    30     0     0     0    'Si 3' 'data/si3.dat'
 14    3    23     0     0     0    'Si 4' 'data/si4.dat'
 14    4     1     1     0     0    'Si 5' ' '
 16    1    33     0     0     0    ' S 2' 'data/s2_23+10lev.dat'
 16    2    41     0     0     0    ' S 3' 'data/s3_29+12lev.dat'
 16    3    38     0     0     0    ' S 4' 'data/s4_33+5lev.dat'
 16    4    25     0     0     0    ' S 5' 'data/s5_20+5lev.dat'
 16    5     1     1     0     0    ' S 6' ' '
 26    1    36     0     0    -1    'Fe 2' 'data/fe2va.dat'
  0    0                               'data/gf2601.gam'
                                       'data/gf2601.lin'
                                       'data/fe2p_14+11lev.rap'
 26    2    50     0     0    -1    'Fe 3' 'data/fe3va.dat'
  0    0                               'data/gf2602.gam'
                                       'data/gf2602.lin'
                                       'data/fe3p_22+7lev.rap'
 26    3    43     0     0    -1    'Fe 4' 'data/fe4va.dat'
  0    0                               'data/gf2603.gam'
                                       'data/gf2603.lin'
                                       'data/fe4p_21+11lev.rap'
 26    4    42     0     0    -1    'Fe 5' 'data/fe5va.dat'
  0    0                               'data/gf2604.gam'
                                       'data/gf2604.lin'
                                       'data/fe5p_19+11lev.rap'
 26    5     1     1     0     0    'Fe 6' ' '
  0    0     0    -1     0     0    '    ' ' '
*
* end
```

File `nst`, described in detail in § 7.10.2, contains the necessary keyword parameters:

```
ND=50,NLAMBD=3,VTB=2.,ISPODF=1,DDNU=50.,CNU1=6.,NITER=0
```

For the testing purposes, this model is not identical to the corresponding model from the BSTAR2006 grid. It is calculated with a lower sampling step in frequency, 50 fiducial Doppler widths, and no iteration (`NITER=0`) of the hybrid CL/ALI scheme is done. This run therefore only initializes the superline cross sections and performs a global formal solution (i.e., a simultaneous solution of the radiative transfer and the kinetic equilibrium equations to obtain new values of mean intensities of radiation and atomic level populations), so it tests most of the features specific to NLTE metal line blanketed models. The user can obviously increase the number of iterations by skipping the `NITER=0` statement, in which case the run would however take several hours.

The first 30 elements, except Li, Be, and B, are included, all with the solar abundances. The model atmosphere includes 11 explicit atoms (H, He, C, N, O, Ne, Mg, Al, Si, S, and Fe), 35 explicit ions, and 1127 explicit NLTE (super)levels. Opacity Sampling is used (ISPODF=1). Unlike the models from the BSTAR2006 grid that were calculated with a sampling step of 0.75 fiducial Doppler width for iron, here we use for simplicity a lower resolution of 50 fiducial Doppler widths. The whole spectrum is represented by 123,396 frequencies. The mean intensity of radiation is linearized at 16 frequencies.

Again, a subdirectory `"./data"`, in which all the atomic data files referred to in the standard input are located, must exist. When using the standard directory tree and the script `RTlusty`, the link to the standard "`data`" directory is done automatically. The model is then run simply as

```
RTlusty  BGA20000g400v2a  BGA20000g400v2
```

where `BGA2000g400v2a` is the core name of the new model, and the second parameter, `BG20000g400v2` sets the file `BG20000g400v2.7` as a starting model for the present run.

Here we also demonstrate the use of the program PRETLUS. It is run as

```
cd $TLUSTY/examples/bstar
ls -s -f $TLUSTY/data  data
$TLUSTY/pretlus/pretlus.exe <BGA20000g40v2a.5
```

The standard output from the program is the following:

```
 MATOM  =      99
 MION   =      35
 MLEVEL =    1127
 MLVEXP =     222
 MTRANS =   20476
 MDEPTH =      50
 MFREQ  =  123396
 MFREQP =  215637
 MFREQC =    4015
```

```
 MFREX  =      16
 MFREQL =    4935
 MTOT   =     241
 MMU    =       3
 MFIT   =     157
 MITJ   =     199
 MMCDW  =       6
 MMER   =       1
 MVOIGT =      79
 MZZ    =       6
 NLMX   =      80
 MSMX   =       1
 MFREQ1 =       1
 MFRTAB =       0
 MTABT  =       0
 MTABR  =       0
 MCROSS =    1132
 MBF    =    1127
 MDEPTC =       0
 MMUC   =       0

parameters in ODFPAR.FOR:

 MDODF  =          3
 MKULEV =       6870
 MLINE  =    1133840
 MCFE   =    7823728
```

This is to be compared to the content of the files `BASICS.FOR` and `ODFPAR.FOR` to check that the actual values of the parameters are greater than or equal to the values listed above. If not, the files `BASICS.FOR` and/or `ODFPAR.FOR` have to be modified accordingly.

6.4 LTE model atmosphere of a K star

Here is an example of using the pre-calculated opacity table, while solving the equation of state on the fly. This example also shows how to deal with convection. The standard input file, called `s4545.5` is as follows:

```
4500. 4.5            ! TEFF, GRAV
 T  T                ! LTE,  LTGRAY
 's45.param'         ! keyword parameters filename
*
* frequencies
*
```

```
 -15000
*
* data for atoms
*
 30                     ! NATOMS
* mode abn modpf
    1   0.      0       ! H
    1   0.      0       ! He
    0   0.      0
    0   0.      0
    0   0.      0
    1   0.      0       ! C
    1   0.      0       ! N
    1   0.      0       ! O
    1   0.      0
    1   0.      0       ! Ne
    1   0.      0
    1   0.      0       ! Mg
    1   0.      0       ! Al
    1   0.      0       ! Si
    1   0.      0
    1   0.      0       ! S
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0
    1   0.      0       ! Fe
    1   0.      0
    1   0.      0       ! Ni
    1   0.      0
    1   0.      0
*
* data for ions
*
*iat   iz   nlevs  ilast ilvlin  nonstd typion  filei
*
   0    0     0     -1      0      0    '    ' ' '
```

The file `s45.param`, described in detail in § 7.10.3, contains the necessary keyword parameters, most importantly `IOPTAB=-1` which sets the mode of eval-

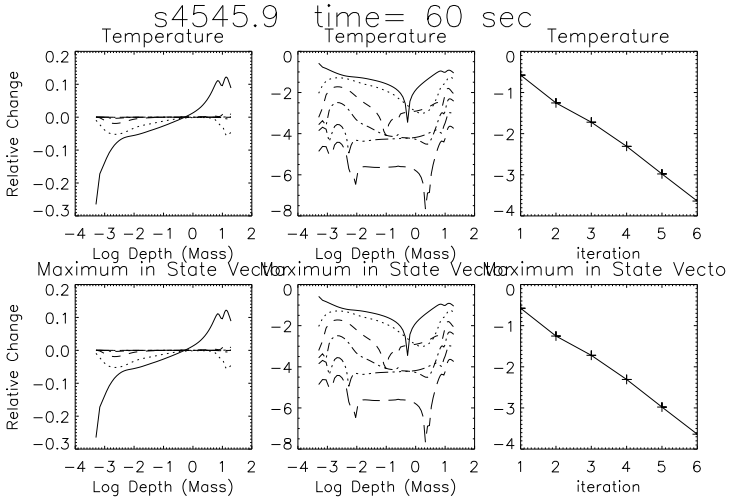

Figure 4: Convergence log for the TLUSTY LTE test-case model for $T_{\rm eff} = 4500$ K and $\log g = 4.5$. Since the Rybicki scheme is used, the maximum relative change of all quantities is equal to the relative change of temperature, so the lower panels are redundant because they are identical to the upper ones.

uation to the pre-calculated opacity table, but solves the equation of state and evaluates the thermodynamic parameters on the fly. The file looks like this:

```
IOPTAB=-1,IFRYB=1,IFMOL=1,IDLST=0
FRCMAX=3.2e15,FRCMIN=1.5e13,IBINOP=0,
ITEK=50,IACC=50
TAUFIR=1.e-7,TAULAS=1.0e2
HMIX0=1,NDCGAP=10,ICONRE=0,IDEEPC=3,CRFLIM=-10
```

The frequency number parameter NFREAD is set to -15000, which sets logarithmically equidistant frequencies between FRCMIN and FRCMAX, which are set in the `s45.param` file. The first 30 elements, except Li, Be, and B, are considered in the equation of state with solar abundances. In this mode, there are no explicit atoms and ions; the input block for ions thus contains only the final line indicating its end.

Due to the specification of the keyword parameters, several additional input files are needed:

`data/absopac.dat` – opacity table (because IOPTAB is set to IOPTAB=-1);
`data/tsuji.molec` – molecular state equation parameters (because IFMOL=1);
`data/irwin.dat` – Irwin partition functions (by default if IFMOL > 0).

Using the standard TLUSTY directory tree, these files are readily available.

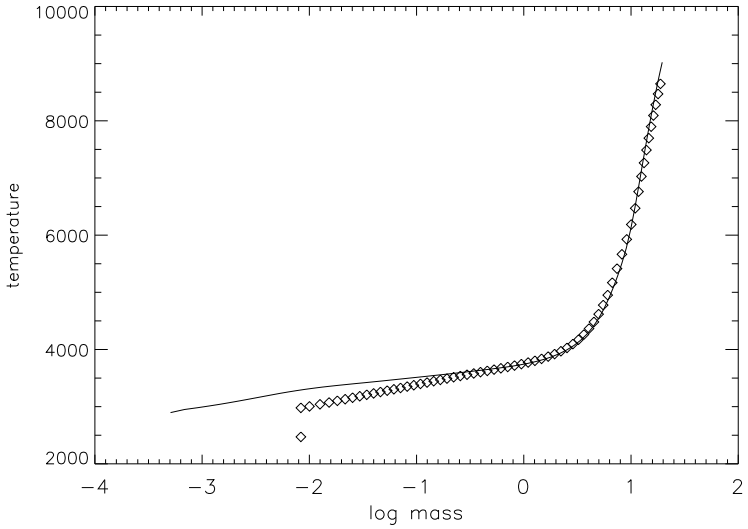

Figure 5: Temperature as a function of column mass for the TLUSTY test-case LTE model for $T_{\rm eff} = 4500$ K and $\log g = 4.5$ (solid line), together with the Kurucz model for the same parameters (diamonds).

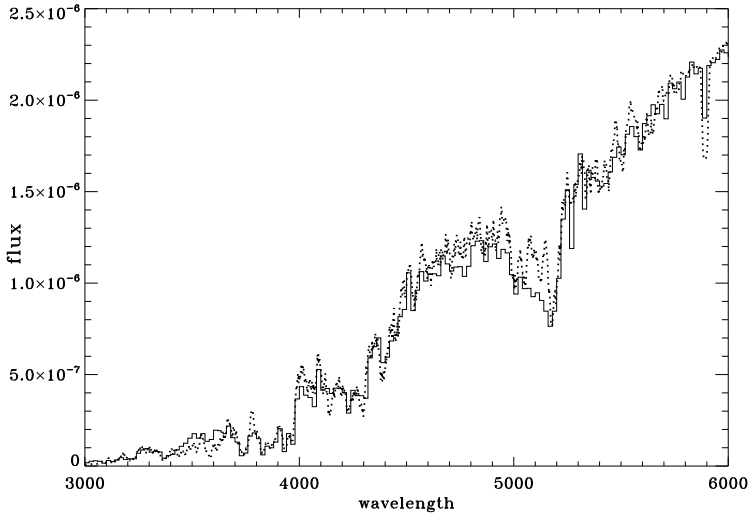

Figure 6: Emergent flux for the TLUSTY test-case model with $T_{\rm eff} = 4500$ K and $\log g = 4.5$, smoothed to about 1Å resolution (dotted line), together with the Kurucz model for the same parameters (solid line histogram).

The convergence of the model is excellent – see Fig. 4. It can hardly be ever better; this is essentially thanks to the use of the Rybicki scheme which linearizes the mean intensities of radiation in all 15,000 frequency points, so the adopted iteration scheme is essentially an exact Newton-Raphson method. The execution was also quite fast; the complete model was calculated in 60 s on a 2.2 GHz Mac. Actually, we used here a binary form of the opacity table; its reading took 20 out of 60 s. When using an ASCII table, the time for its reading increases to about 50s.

In Fig. 5, we plot the temperature structure, together with the temperature structure of the Kurucz model with the same $T_{\rm eff}$ and $\log g$. Overall temperature structure is quite similar, but there are small differences, in particular close to the surface. They are most likely caused by our neglecting the contribution of molecules in the opacity table. We stress that the current opacity table is not meant to provide the exact opacity, but rather to be used for testing purposes.

Figure 6 shows an analogous comparison of the emergent flux. Again, an agreement between the two models is quite good, in particular in view of the fact that our opacity table is just a beta-version of a more complete opacity table that is currently under construction.

6.5 Moderately cool DA white dwarf

We take an example of a DA (pure-hydrogen) white dwarf with $T_{\rm eff} = 10,000$ K and $\log g = 8$. The atmosphere is convective; we assume the ML2-type convection with the mixing length equal to 0.6 pressure scale height. Hydrogen line broadening is treated using the Tremblay tables (see § 12.1.1). The standard input for an LTE model is as follows (file `t100g80l.5`):

```
  10000.0      8.0
  T    T
  'cwd.flag'
  200
*
* data for atoms
*
       1
* mode abn modpf
    2   0   0
*
*iat iz  nlv  ilst ilvln nonst typion  filei
*
 1    0   16    0    0    0   ' H 1' './data/h1s16.dat'
 1    1    1    1    0    0   ' H 2' ' '
 0    0    0   -1    0    0   '    ' ' '
```

The keyword parameter file `cwd.flag` given as

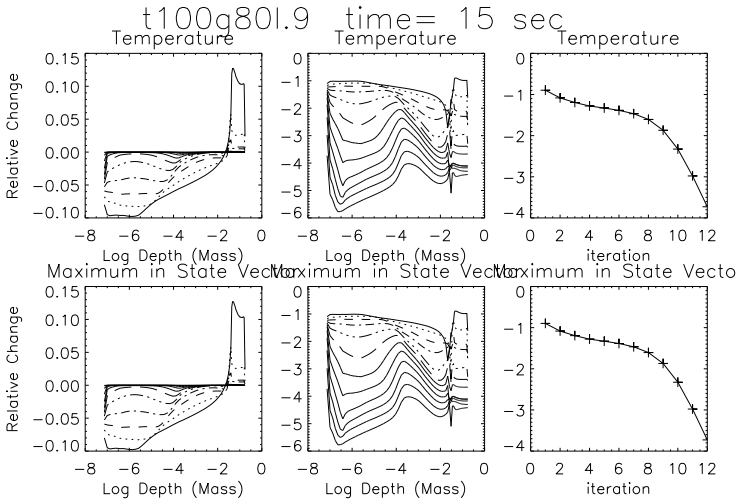

Figure 7: Convergence log for the TLUSTY test-case LTE model of a DA white dwarf with $T_{\rm eff} = 10,000$ K and $\log g = 8$.

```
IFRYB=1,IHYDPR=2
IPRINT=3,ITEK=40,IACC=40
TAUDIV=1.e-2,IDLST=0
HMIX0=0.6,MLTYPE=2,IMUCON=40,ICONRS=5
NDCGAP=5,ICONRE=0,IDEEPC=3,CRFLIM=-10.
```

Due to the specification of the keyword parameters, one needs the additional file `data/tremblay.dat`. Again, the model is run as

```
RTlusty t100801
```

The convergence pattern is displayed in Fig. 7. The convergence is very smooth; this is essentially due to to using the Rybicki scheme, and because of employing special procedures to treat convection in the global formal solution as described in Paper II, Appendix B2.

NLTE effects are not expected to be crucial, but to verify this statement it is necessary to compute the corresponding NLTE model. The standard input (file `t100g80n.5`) is very similar to the LTE input file, with the first three lines being now

```
      10000.0       8.0
  F     F
'cwdn.flag'
```

with the keyword parameters file `cwdn.flag` is a slightly modified `cwd.flag`, namely

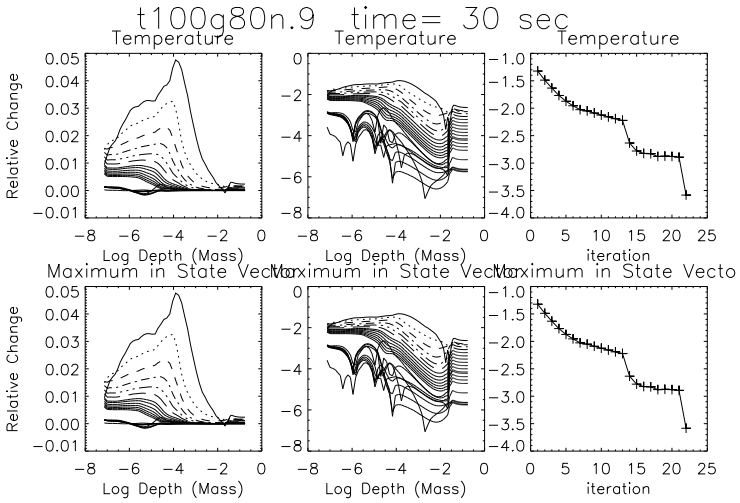

Figure 8: Convergence log for the TLUSTY test-case NLTE model of a DA white dwarf with $T_{\rm eff} = 10,000$ K and $\log g = 8$.

```
IFRYB=1,IHYDPR=2
IPRINT=3,ITEK=20,IACC=14
TAUDIV=1.e-2,IDLST=0
HMIX0=0.6,MLTYPE=2
NDCGAP=5,ICONRE=0,IDEEPC=3,CRFLIM=-10.
IMUCON=40,ICONRS=5
```

The most interesting feature is that one is able to converge the model while still using the Rybicki scheme. Not only it works well in this case, but in fact it works significantly better than the original hybrid CL/ALI scheme, which is surprisingly difficult to converge. The reason for one can use the Rybicki scheme at all is that departures from LTE are not very large, and the reason for its stability is that it represents an essentially exact Newton-Raphson scheme without an ALI treatment of the radiation field in any frequency. The reason why the original CL/ALI scheme has problems is that the energy balance, represented here by the radiative/convective equilibrium, leads to a steep temperature gradient, which is hard to converge if some quantities are lagged behind.

The model is run simply by

```
RTlusty t100g80n t100g80l
```

The convergence pattern is shown in Fig. 8. The convergence is relatively slow, but stable. We see a significant effect of the Ng acceleration, which is first applied in the 14th iteration, and then after each 4 iterations. Usually, one does

not apply Ng acceleration for models with convection, but in this case its use is warranted because the atmospheric structure in deep layers, where convection is present, is not expected to be influenced by NLTE effects to any significant degree.

6.6 Accretion disk around a white dwarf

The standard input for a simple H-He model of the vertical structure of an accretion disk around a white dwarf, analogous to the simple model atmosphere computed in § 6.2, is as follows (file `d1lt.5`):

```
 0.8 1.e-9  0.01 2        ! XMSTAR,XMDOT,RSTAR,RELDST
 T  T                     ! LTE, LTGRAY
 'param'                  ! keyword parameters file
*------------------
* frequencies
 50                ! NFREAD
*------------------
* data for atoms
*
 8                 ! NATOMS
* mode abn modpf
    2   0   0
    2   0   0
    0   0   0
    0   0   0
    0   0   0
    1   0   0
    1   0   0
    1   0   0
*-----------------
* data for ions
*
*iat    iz   nlevs  ilast ilvlin  nonstd typion  filei
*
   1     0     9      0    100      0    ' H 1' './data/h1.dat'
   1     1     1      1      0      0    ' H 2' ' '
   2     0    14      0    100      0    'He 1' '/data/he1.dat'
   2     1    14      0    100      0    'He 2' '/data/he2.dat'
   2     2     1      1      0      0    'He 3' ' '
   0     0     0     -1      0      0    '    ' ' '
*
* end
```

and the keyword parameter file `param` is simply

```
ALPHAV=0.3
```

Important note: To tell TLUSTY that an accretion disk model is computed, one has to create a file `fort.1` with just one number, 1.

This run computes an LTE model (from scratch) of a ring of an accretion disk around a star with mass 0.8 solar masses and radius $0.01R_\odot$ (a typical white dwarf), and with a mass accretion rate $\dot{M} = 10^{-9}\ M_\odot$/year, and at a distance 2 stellar radii. The viscosity parameter is set to $\alpha = 0.3$.

An essentially identical model is obtained replacing the first line of the standard input file with

```
0.  35165.  3.934e-2  5.742e1       ! TEFF, QGRAV, DMTOT
```

Here, as explained in § 4.1, the central star mass is set to 0, in which case the following three parameters have the meaning of the effective temperature $T_{\rm eft}$ (TEFF), gravity acceleration parameter Q (QGRAV), and the total column mass m_0 (DMTOT). These parameters can be found at the beginning of the standard output file of the previous run. In this case the parameter α is not needed (because it is used only to evaluate the total column mass), so that the keyword parameter file `param` can be empty. However, since α is not used, its value set up in `param` is inconsequential, and therefore the run may be done with the file `param` unchanged.

One can also continue on and construct NLTE/C and NLTE/L models, exactly as in the case of a simple H-He atmosphere of § 6.2. When this is done, one finds that the departures from LTE are much smaller now because of much higher effective gravity acceleration (that is, g is large everywhere except very close to the midplane), and the corresponding high density of the material.

7 Keyword parameters

7.1 General description

There are over 210 individual keyword parameters. We stress that a keyword, or optional, parameter is defined as such for which the program assigns a default value that is meant to provide an optimum value for most applications, or the most reasonable value. A small number of keyword parameters are actual physical parameters, like the convective mixing length or the turbulent velocity, which are set to zero for most applications. However, the majority of keyword parameters are various computational flags and switches that specify a detailed setup of the numerical method. Notice that the overall degree of sophistication of the resulting model atmosphere is determined by the atomic input files, described in Chap. 11. The keyword parameters discussed in this section, with the exception of the physical parameters mentioned above, will mostly influence the numerical performance, such as the rate of convergence (or a lack thereof!), the total computer time, the numerical accuracy, the degree of auxiliary output, etc.

The file, whose name is specified by the standard parameter FINSTD (see § 4.1), contains a list of the keyword parameters to be changed from their default 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: comma (`,`), 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 has to 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 1986); we have used and modified his routines GETWRD and RINPUT.

Hint: Since parameters to be changed have 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 then easily be reinstated later. For instance, coding

`ITEK=8`

has the effect of starting the Kantorovich acceleration (see Sect.7.4.8) at the 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 this section, we will describe only the most important parameters. The less important, very specific, or rarely used parameters are described in Part II in Chaps. 12 and 13.

7.2 Input physical parameters

Most basic physical parameters ($T_{\rm eff}$, $\log g$, chemical abundances; and basic parameters for a ring in an accretion disk) are set up by the standard input file. However, there are some physical parameters which are being set by corresponding keyword parameters. We list them below.

7.2.1 Universal 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 (essentially, to check for the convective stability of the resulting model);
- < 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} (if $< 10^3$) or cm s^{-1} (if $\geq 10^3$).
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 $P_{\rm turb} = (1/2)\rho v^2_{\rm turb}$

DEFAULT: IPTURB=1.

7.2.2 White dwarf–specific parameters

They account for equilibrium diffusion of helium and thus 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.

7.2.3 Accretion disk–specific parameters

ALPHAV – the viscosity parameter α.
- > 0 – the numerical value of α;
- ≤ 0 – the viscosity is set through the Reynolds number.

DEFAULT: ALPHAV=0.1

REYNUM – the Reynolds number. It takes an effect, and the viscosity is evaluated through the Reynolds number, only if the keyword parameter ALPHAV is set to zero or a negative value.
DEFAULT: REYNUM=0.

IVISC – a mode of treating depth-dependent viscosity:
- ≥ 0 – the depth-averaged viscosity is determined through the "averaged" α, given by the parameters ALPHAV. By default, the local kinematic viscosity is constant, but can also be treated as a two-step power law as

described by Hubeny & Hubeny (1998). In this case, one needs to employ four more keyword parameters, as described in § 12.8.
• < 0 – the local viscous stress is given by $t_{\phi r} = \alpha P_{\rm gas}$; i.e. α determines the *local* viscosity.
DEFAULT: IVISC=0

7.3 External irradiation

External irradiation brings complications into the methodology of computing model stellar atmospheres because it breaks several fundamental assumptions of the adopted modeling procedure. First, it generates departures from horizontal homogeneity. Second, it involves a dependence of specific intensity not only on the azimuthal angle, but also on the polar angle.

There is a special variant of TLUSTY, briefly described in Sudarsky et al. (2005), that is able to deal with a full angular dependence of the external irradiation. The corresponding calculations are, however, quite time-consuming even if one employs a powerful ALI-based numerical scheme for solving the radiative transfer equation. Experience shows that such detailed calculations are necessary only in special cases, for instance for strongly irradiated extrasolar giant planets.

The mainstream TLUSTY therefore adopts a simpler approach. One replaces a highly anisotropic irradiation by an isotropic radiation intensity that gives the same total incoming energy. The irradiated intensity is taken either as hoc, as a diluted black-body spectrum, or through a theoretical flux from an actual model atmosphere. In that case, the dilution factor is either set up to a specific value (either an empirical one, or that obtained by independent calculations), or is given through the radius and distance of the irradiating object. In the present version, the irradiating object is assumed to be a spherical star.

To deal with departures from the horizontally homogeneous approximation, one can either construct several model atmospheres for varying distances from the substellar point (the point on the surface of the irradiated star at which the external irradiation comes in the direction of the normal to the surface), or to assume that the irradiated intensity is spread over the surface of the irradiated star. One then introduces a factor f that represents the ratio between the specific intensity at the substellar point and the specific intensity that is characteristic of the averaged irradiation over the whole irradiated hemisphere. Assuming a homogeneous distribution of energy gives $f = 1/2$, but it turned out (see Burrows et al. 2008) that the most appropriate value is $f = 2/3$.

The external specific intensity is given by

$$I_\nu^{\rm irrad} = W H_\nu^* \tag{1}$$

where H_ν^* is the Eddington flux (the first moment of the specific intensity) at the surface of the irradiating object (star), in erg cm^{-2} s^{-1} Hz^{-1}. The reason for using the Eddington flux is that most stellar atmosphere programs and model grids (TLUSTY; Kurucz) provide H_ν to represent the emergent spectrum. The

dilution factor in this case is given by

$$W = f(1/2)(R^*/d)^2, \tag{2}$$

where the factor $1/2$ comes from the the conversion of H to I, see Eq. (7) of Paper II.

Here is a list of keyword parameters that control the treatment of irradiation:

TRAD – a switch for treating the external irradiation:

- $= 0$ – no external irradiation is considered;
- > 0 – the external irradiation is considered; the irradiated intensity of radiation is assumed to be given by Eq, (1), $I_\nu^{\rm irrad} = W B_\nu(T^*)$, 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^*. This is a general option, which may mimic for instance an irradiation from a distributed source. In the special case of an irradiation by a spherical star, T^* is given by the effective temperature of the irradiating star.
- < 0 – the irradiated intensity at the top of the atmosphere is given by the emergent spectrum of the source of irradiation, Eq. (1), where the Eddington flux H_ν, in erg cm^{-2} s^{-1} Hz^{-1}, is read from a special input file `source.flux`.

  The quantity abs(TRAD) then represents the number of frequency points in the file `source.flux`. These frequencies can be arbitrary; the program then interpolates to the frequency points used by TLUSTY.

  The dilution factor W is given either through the parameter WDIL, or is computed using the radius of the irradiating star, R^* (given by keyword parameter RSOURC), the distance between the modeled object and the irradiation source, d (parameter ADIST), and the spreading factor f (parameter SPRFAC) – see below.

  DEFAULT: TRAD=0.

WDIL – the dilution factor W, used either for TRAD > 0, or for TRAD < 0 if the parameters RSOURC and ADIST are not set.
DEFAULT: WDIL=1.

RSOURC – the radius if the irradiating star. Can be expressed either in cm, or in the units of solar radii. It takes effect only for TRAD < 0.
DEFAULT: RSOURC=0.

ADIST – distance between the center of the irradiating star and the top of the irradiated atmosphere. It can be expressed either in cm or in Astronomical Units. It takes effect only for TRAD < 0.
DEFAULT: ADIST=0.

SPRFAC – spreading factor f used in Eq. (2). It takes effect only for TRAD < 0.
DEFAULT: SPRFAC=0.667

7.4 Basic numerical setup parameters

7.4.1 Global setup

These are potentially very important parameters that in fact determine the overall mode of calculation of a model atmosphere.

IFRYB – a switch for invoking the Rybicki scheme:
- $= 0$ – original hybrid CL/ALI scheme is used
- ≥ 1 – Rybicki scheme is used

DEFAULT: IFRYB=0

ISPODF – the basic mode of treating line blanketing:
- $= 0$ – a classical option – line blanketing is either not considered, or treated through the (obsolete) Opacity Distribution Function (ODF) option. The frequency points are set up for each line (or ODF) separately. Lines are assumed to have a Doppler or Voigt profile. The regions between lines are represented by a small number of frequency points, set up through input parameter NFREAD, and additional keyword parameters – see § 7.4.2.
- ≥ 1 - the Opacity Sampling (OS) mode. Frequencies are set up systematically with a variable step depending on the kind of opacity source to be represented. Small frequency steps are adopted to sample adequately lines of light elements. The regions in between these lines and the iron-peak lines are sampled with a step DDNU times the fiducial Doppler width. For details refer to § 7.7.

IOPTAB – a switch specifying the use of pre-calculated opacity tables:
- $= 0$ – classical option – no pre-calculated opacity table is used;
- < 0 – all opacities are calculated by means of a pre-calculated opacity table. In this case, one does not specify any explicit atoms, ions, and levels. Only LTE models can be computed with this option.
- $= -1$ – in addition, equation of state and thermodynamic parameters are computed on the fly.
- $= -2$ – in addition, also equation of state and thermodynamic parameters are given by pre-calculated tables.
- > 0 – hybrid option – one still selects explicit atoms, ions, and levels, for which the opacity is computed on the fly, while for remaining species one uses an appropriate pre-calculated opacity table.

DEFAULT: IOPTAB=0

IFMOL – a switch for including molecular formation in the equation of state.
- $= 0$ – molecular formation neglected
- > 0 – molecules are included in the equation of state, as described in Paper II, § 2.7.

DEFAULT: IFMOL=0

ICOMPT – a switch for including Compton scattering. In this case, several other keyword parameters take effect – see § 12.5.

• = 0 – Compton scattering is not included; electron scattering is treated as Thomson (coherent) scattering;
• > 0 – Compton scattering is included.
DEFAULT: ICOMPT=0

7.4.2 Setup of frequency points

FRCMAX – the maximum frequency $\nu_{\max}$.
• = 0 – maximum frequency is set up such as:
(a) for atmospheres: $\nu_{\max} = 8 \times 10^{11} T_{\rm eff}$; i.e. $h\nu_{\max}/kT_{\rm eff} \approx 38$;
(b) for accretion disks: $h\nu_{\max}/kT_{\rm mid} = 17$, where $T_{\rm mid}$ is the local temperature at the midplane, evaluated approximately through the effective temperature and the total column density Σ as $T_{\rm mid} = 2.83{\times}10^{11}\, T_{\rm eff}\, (0.2\,\Sigma)^{1/4}$ (see Hubeny et al. 2001).
• > 0 – the value of maximum frequency.
DEFAULT: FRCMAX=0.

CFRMAX – an auxiliary parameter for setting the maximum frequency.
• = 0 – the value of $\nu_{\max}$ given by FRCMAX is unchanged;
• > 1 – the value of $\nu_{\max}$ is set to the maximum of the one given by FRCMAX and CFRMAX times the frequency of the explicit photoionization edge with the highest-frequency.
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 the minimum frequency.
DEFAULT: FRCMIN=10^{12}

FRLMAX – the maximum frequency in the line transitions. If the central frequency of a line is larger than FRLMAX, the line is neglected.
• = 0 – the maximum frequency in line transitions is set to FRCMAX.
• > 0 – the value of maximum frequency in 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 setting of frequency points in the high-frequency tail.
• > 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. 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 NFREAD. This option is very useful if there are many explicit levels which would generate an unnecessarily large number of frequencies around completely unimportant edges.
DEFAULT: NFTAIL=21

DFTAIL – see above.
DEFAULT: DFTAIL=0.25

7.4.3 Setup of the radiative transfer equation and ALI

ISPLIN – Mode of numerical representation of the radiative transfer equation (for details see Paper II, § 3.8.1)
• $= 0$ – standard second-order Feautrier scheme
• $= 1$ – spline collocation scheme
• $= 2$ – Auer's fourth-order Hermitian scheme
• $= 3$ – Rybicki–Hummer improved Feautrier scheme
• $= 5$ – Discontinuous Finite Element (DFE) scheme
DEFAULT: ISPLIN = 0

IFALI – basic switch for treating the radiative transfer equation for frequency points that are treated with ALI in the hybrid CL/ALI method:
• $= 0$ – no ALI option, i.e. all frequency points are explicitly linearized. All transition that are not selected for linearization are treated using the "fixed-rates" option (essentially an ordinary Lambda iteration) 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.
• $= 5$ – ALI scheme with diagonal Λ^* is used for frequency points treated within the ALI method;
• $= 6$ – ALI scheme with tri-diagonal Λ^*. This option was not fully tested in version 205; and does not work properly for some setups. It is not recommended.
DEFAULT: IFALI=5

JALI – switch determining the type of evaluation of the Λ^* operator.
• $= 1$ – Λ^* evaluated by the Rybicki-Hummer (1991) algorithm;
• $= 2$ – Olson-Kunasz (1987) algorithm.
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 (thus overwriting a specific input for line transitions in an atomic data file);
• = 2 – all frequency points altogether are set to the ALI mode (i.e. the fully ALI scheme is forced regardless of other input).
• = −1 – all points are in the linearized mode, regardless of other input (i.e., the original complete linearization method).
DEFAULT: IFRALI=0

RADZER – a 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 the mean intensity decreases below RADZER times the maximum relative intensity, it is set to zero, and the radiative transfer equation is written and linearized as $J_\nu = 0$.
DEFAULT: RADZER=1.e-20

7.4.4 Setup of the kinetic 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 refers 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 the default anyway).
• = 0 – IATREF is set to 1 (i.e. the first explicit species).
DEFAULT: IATREF=1

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

POPZER – a value of the ratio of a level population over the population of the most populated level of a given species, below which the population is declared to be "too small" and is set to 0. This option allows to consider many ionization degrees of an atom without running into numerical problems connected with too small/large numbers.
DEFAULT: POPZER=1.e-20

NITZER – iteration number till which the population can be zeroed or unzeroed. 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=1

7.4.5 Setup of the radiative equilibrium equation

NDRE – a parameter that defines the treatment of the radiative equilibrium equation, 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 d, $d = 1, \ldots$,ND−IDLST

– the differential form is used for depth points where the Rosseland optical depth is greater than TAUDIV.

The coefficients α and β in Eqs. (16) or (19) of Paper II are thus given by

$$\alpha_d = 1 \quad \text{for} \quad d \leq \text{IDLST}, \quad \alpha_d = 0 \quad \text{elsewhere},$$
$$\beta_d = 1 \quad \text{for} \quad \tau_{\text{Ross}} > \tau_{\text{div}}, \quad \beta_d = 0 \quad \text{elsewhere},$$

• > 0 – the coefficients are step functions with discontinuity at $d =$ NDRE, i.e.:

– for depth points ($d = 1, \ldots$,NDRE−1) – purely integral form ;

– for depth points ($d =$NDRE,. . .,ND) – purely differential form.

This option is outdated and is not recommended. Much better option is the previous one, NDRE=0.

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

NRETC – a switch for setting a fixed temperature at the upper layers

• = 0 – no fixed temperature; radiative equilibrium is solved for all depths

• > 0 – the temperature at the first NRETC depth points is held fixed (given by the input model); radiative equilibrium at those depths is not solved for the temperature.

DEFAULT: NRETC=0

7.4.6 Discretization and linearization loop control

ND – number of depth points
DEFAULT: ND=70

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

NITER – maximum number of global iterations of the linearization scheme.
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 iterations for the global formal solution; which typically consists of solving the coupled radiative transfer and kinetic equilibrium equation. Historically, these were ordinary Lambda iterations, hence the name NLAMBD. Currently the default procedure is instead the ALI scheme with preconditioning.
DEFAULT: NLAMBD=2 for NLTE; NLAMBD=1 for LTE models

CHMAXT – a parameter which enables to change the number of iterations of the global formal solution (NLAMBD) when the model is almost converged. If the maximum of the absolute values of the relative changes of 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 iterations of the global formal solution – see above.
DEFAULT: NLAMT=1

7.4.7 Setup of the linearization matrices

Each of the following parameters: INHE, INRE, INPC, INSE, INMP, INDL, INZD, corresponds to one equation and one model parameter, as described below.

If INxx = 0, then the corresponding equation is not solved, and the corresponding quantity is not a component of the state vector. Instead, it is held fixed to the values from the starting model.

If INxx > 0, the corresponding equation is solved, and the corresponding quantity is the (NFREQE+INxx)-th component of the vector ψ of unknown model parameters (the first NFREQE components are mean intensities of radiation in the explicitly linearized frequency points). In the following, by "the position" we mean the position of the corresponding quantity in the state vector after the first NFREQE quantities.

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

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

INPC – the position of n_e; the index of the charge conservation equation (or the number 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 – the position of n_1, i.e. the first population; index of the first kinetic equilibrium equation.
DEFAULT: INSE=4 (or INSE=5 for convective models or disks)

INMP – the position of $n_{\rm m}$ – massive particle number density; after Auer & Mihalas (1969). This option is included for historical reasons only.
DEFAULT: INMP=0

INDL – the position of ∇ – 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. This is done if IFIXMO is set to a non-zero value.
DEFAULT: IFIXMO=0

7.4.8 Acceleration parameters

IACC – a switch for the Ng acceleration procedure:
- ≤ 4 – Ng acceleration is done in the 7th, 11th, etc, iteration;
- ≥ 5 – Ng acceleration is done in the iterations ITER=IACC, IACC+IACD, IACC+2×IACD, etc.
- ≤ 0 – no Ng acceleration.

DEFAULT: IACC=7

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

KSNG – if set to 1, one excludes populations of all levels except ground states and the highest ions from contributing to evaluating the acceleration parameters. In other words, these populations have weights $W_{di} = 0$ in Eq. (140) of Paper II.
DEFAULT: KSNG=0

ITEK – the iteration after which the Kantorovich method is set up.
DEFAULT: ITEK=4

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

7.5 LTE-gray model input

7.5.1 Stellar atmospheres

TAUFIR – the Rosseland optical depth in the first depth point.
DEFAULT: TAUFIR = 10^{-7}

TAULAS – the Rosseland optical depth in the last depth point.
DEFAULT: TAULAS $= 3.16 \times 10^2$

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

IPRING – a flag that controls the diagnostic output (to the standard output file, unit 6) 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 (for convective models).
DEFAULT: NCONIT=10

ICHANM – a switch to setting the mass scale of the LTE-gray model in the convection zone.
- $= 0$ – the column mass scale that follows from the first estimate of the model without convection is held fixed;
- > 0 – the column mass scale is recalculated from $\tau_{\rm ross}$ and the current $\chi_{\rm ross}$ that already takes into account a change of the structural parameters (T, $n_{\rm e}$) due to the presence of convection.

DEFAULT: ICHANM=1

7.5.2 Accretion disks

For details of the physical and the mathematical formulation, see Paper II, § 4.2.

DM1 – the column mass in the first depth point.
DEFAULT: DM1 $= 10^{-3}$

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

ABPMIN – the floor value of the Planck mean opacity. That is, the Planck mean opacity is set to the maximum of computed Planck mean and the value of ABPMIN. It is introduced to avoid spuriously low values of the Planck mean opacity at the initial stages of computation.
DEFAULT: ABPMIN $= 10^{-5}$

ABROS0 – the initial estimate of the Rosseland opacity (per gram) at the first depth point – the same as in the case of stellar atmospheres.
DEFAULT: ABROS0 = 0.4

IDMFIX – a switch for setting the characteristic temperature for evaluating the sound speed and the gas and radiation pressure scale heights when computing the starting LTE-gray model.
• $= 1$ – the characteristic temperature is set to the effective temperature;
• $\neq 1$ the characteristic temperature is set to T_1, the temperature at the first depth point, which is determined iteratively – see § 12.8.
DEFAULT: IDMFIX=1

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

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

TDISK – if set to positive value, it has the meaning of the temperature of the disk, assumed constant with height. This provides a means to compute the hydrostatic structure of an isothermal disk. Otherwise, the temperature structure is determined by solving the energy balance equation.
DEFAULT: TDISK=0

7.6 Parameters for modifying the starting input model atmosphere

INTRPL – a switch indicating that the input model atmosphere has to be interpolated to a new depth scale to serve as a starting model for the current run. For a detailed discussion, see Chap. 8.
• $= 0$ – no interpolation; i.e. the same depth grids are used in the input and the current models;
• > 0 – the input model is interpolated to a new depth grid. 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 Chap. 8.
• $= 0$ – 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 current model to be computed);
• > 0 – a "simple" change of the level structure – levels are only added, and only for new species. Starting populations of the new levels are computed in LTE;
• < 0 – change of the structure; a detailed additional input for each level

of the present run is required.
DEFAULT: ICHANG=0

7.7 Line blanketing

ISPODF – the basic mode of treating line blanketing:

- $= 0$ – line blanketing, described through the concept of superlevels and superlines, is either not considered, or is treated in the Opacity Distribution Function (ODF) mode (which is still offered by TLUSTY, but is obsolete). Here, frequencies are set up for each line or ODF. The corresponding 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 the lines of light elements adequately. In between these lines, iron-peak lines are sampled with a step DDNU times the fiducial Doppler width 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 the gf-value. Parameter STRLX sets the selection criterion (the smaller STRLX the more lines are selected; values $10^{-6} \leq \mathrm{STRLX} \leq 10^{-10}$ are generally appropriate). The cross sections are recalculated after the 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 the layer where $T \approx T_{\rm eff}$) 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 case ISPODF=0 is appropriate. However, we stress that for computing fully blanketed models the option ISPODF=1 (the Opacity Sampling approach) is preferable.

  DEFAULT: ISPODF=0

DDNU – the step for the 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 $\nu_{\rm max} = \texttt{CNU1} \times 10^{11} \times T_{\rm eff}$. Frequencies for Opacity Sampling are set up from $\nu_{\rm max}$ to lower frequencies, or from the highest bound-free limit if this limit exceeds $\nu_{\rm max}$.
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 $\nu_{\rm min} = 3.28805\,10^{15}/\texttt{CNU2}^2$.
DEFAULT: CNU2=3.

STRLX – selection criterion for iron-peak element 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 superlines are computed and stored.
• $= 0$ – sets the default of 3 depths (with depth indices $ID = 1, ND$, and the depth where $T \approx T_{\rm eff}$);
• > 0 – number of depths. Their indices are set equidistant between 1 and ND (including these).
DEFAULT: JIDS=0

7.8 Treatment of convection

ICONV – a flag to switch on convection:
• $= 0$ – convection is neglected. However, if the keyword 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 obsolete. The user is recommended to use the 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 it is not linearized.
DEFAULT: ICONV=0

ICONRE – if set to a positive value, subroutine CONREF is called that recalculates temperature in the convection zone between the individual iterations of the global linearization scheme, using the procedure specified in Paper II, Appendix B2. ICONRE has the meaning of the iteration number till which the correction procedure is being performed. However, the correction is done only at depth points where the convective flux exceeds a certain fraction of the total flux, given by the parameter CRFLIM. Usually, this routine helps significantly; there may however be cases when it does not help. The symptom of this problem 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

ICONRS – a similar switch for the starting iteration number in which the correction procedure CONREF is performed.
DEFAULT: ICONRS=10

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

IMUCON – a switch for invoking an additional temperature correction procedure, defined by Eq. (343) of Paper II, Appendix B2, on top of the standard one that is set up through the keyword parameters ICONRE and ICONRS. It takes effect only if ICONRE > 0 (that is, if a correction is done at all).
• $= 0$ – no additional correction procedure;
• > 0 – an additional correction procedure is performed at the global iteration starting with iteration number IMUCON.
DEFAULT: IMUCON=10

If ICONRE is set to a positive value, then there are two 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 ($\nabla > \nabla_{\rm ad}$), but for which the current values lead to $\nabla < \nabla_{\rm ad}$ and thus are viewed as convectively stable (this may happen during a global iteration process because in the convection zone ∇ is always very close to $\nabla_{\rm ad}$, and the linearization may easily lead to ∇ slightly smaller than $\nabla_{\rm ad}$). Moreover, the actual value of IDEEPC controls the treatment of the deepest layers of the atmosphere:
• $= 0$ – convection gaps are not considered; the temperature correction procedure is performed only in the layers with $\nabla > \nabla_{\rm ad}$.
• $= 1$ – convection gaps are considered as described above, but the position of the convection zone in the deepest layers is left as specified by the current values of ∇ and $\nabla_{\rm ad}$.
• ≥ 2 – 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.
• $= 3$ – the end of convection zone is reset to ND regardless of where it currently ends.
• $= 4$ – 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 convection instability condition $\nabla > \nabla_{\rm ad}$ 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 the procedure 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.

7.9 Artificial truncation of the radiation pressure

The reason for considering a truncation of radiation pressure is to avoid numerical as well as physical instability on the surface layers of hot stars. In this case the true radiation pressure may exceed the gas pressure, leading to an onset of stellar wind, which cannot be treated by TLUSTY. However, it is still quite meaningful to construct hydrostatic model photospheres for the deeper layers of such stars, for which the hydrostatic equilibrium is an excellent approximation, and where most of the observed spectral features (except strongest lines) do originate. A more detailed discussion of this topic is presented in Lanz & Hubeny (2003).

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.

IFPRAD – a switch for turning off the radiation pressure completely.
• $= 0$ – radiation pressure is set to zero everywhere;
• > 0 – radiation pressure is considered (but still may be limited by means of the keyword parameter XGRAD).
DEFAULT: IFPRAD=1

7.10 Examples

Now we take the examples of files with keyword parameters that were considered in Chap. 6 and explain in more detail their contents and the reasons for the adopted settings.

7.10.1 Simple H-He model atmosphere in § 6.2

In this case, the standard input file sets the name of the keyword parameter file FINSTD to a null string. in which case no keyword parameters were set, and thus all assume their default values. Recapitulating the basic features of the standard, default setup:
• model is computed by the hybrid CL/ALI method, with Kantorovich acceleration started in the 4th and Ng acceleration in the 7th global iteration;
• no superlines, no convection, no molecules, and no additional opacities.

7.10.2 NLTE line-blanketed model of a B star in § 6.3

The keyword parameter file `nst` (with the name specified in the standard input) has the following content:

```
ND=50,NLAMBD=3,VTB=2.,ISPODF=1,DDNU=50.,CNU1=6.,NITER=0
```

which have the following meaning:
• ND=50 – sets the number of depth points to 50. It is lower than the default value ND=70, and was used in our `ostar2002` and `bstar2006` model grids because: (i) the overall accuracy of the model is only insignificantly lower than for 70 depth points; (ii) the convergence of the ALI (and thus the hybrid CL/ALI) scheme is somewhat faster; and (iii) for practical reasons, namely that setting ND=50 (and also MDEPTH=50 in the "INCLUDE" file `BASICS.FOR`) decreases the memory of consumption significantly, considering that line-blanketed models need a large amount of memory for computing superline cross sections due to the required large values of parameters `MKULEV`, `MLINE`, and, in particular `MCFE`

in the "INCLUDE" file `ODFPAR.FOR`. If the core memory is no longer an issue, one could calculate models with default ND=70 or with an even higher value of ND.

• NLAMBD=3 – sets the number of internal iterations in the global formal solution to 3. This choice leads to a more stable overall iteration process. Having more iterations would improve the global convergence properties even more, but the formal solution would be more time-consuming. The adopted value of 3 represents a reasonable compromise.

• VTB=2. – set the turbulent velocity to 2 km/s

• ISPODF=1 – the basic parameter that sets the calculation of a line-blanketed model with treating the superline cross sections in the OS (Opacity Sampling) approach.

• DDNU=50. – sets the sampling step to 50 fiducial Doppler width. This is a lower resolution that was used in BSTAR2006 grid, where DDNU=0.75 was used.

• CNU1=6. – specifies the highest frequency for which are the superlines consdired, as explained in § 7.7.

• NITER=0 – sets the number of the linearization iterations to zero; that is, only an initialization and the first formal solution is performed.

7.10.3 LTE model atmosphere of a K star in § 6.4

The content of the keyword parameter file `s45.param` is as follows

```
IOPTAB=-1,IFRYB=1,IFMOL=1,IDLST=0
FRCMAX=3.2e15,FRCMIN=1.5e13,IBINOP=0,
ITEK=50,IACC=50
TAUFIR=1.e-7,TAULAS=1.0e2
HMIX0=1,NDCGAP=10,ICONRE=0,IDEEPC=3,CRFLIM=-10
```

which has the following meaning:

• IOPTAB=−1 – sets the mode of evaluation of opacities to using the precalculated opacity table, but with solving the equation of state and evaluating the thermodynamic parameters on the fly.

• IFRYB=1 – sets the global iteration method to the Rybicki scheme. For LTE models of cool stars, and in particular when convection is present, this scheme works much better than the standard hybrid CL/ALI scheme as it is more stable, and the convergence rate is much faster.

• IFMOL=1 – stipulates that molecules are included in the equation of state (as is of course mandatory for such low temperature models).

• IDLST=0 – sets the proper treatment of the energy equation at the lower boundary. This option has to be used in conjunction with IFRYB=1.

• FRCMAX, FRCMIN – sets the minimum and maximum frequency.

• IBINOP=0 – signifies that the opacity table is an ASCII file. The default value of the parameter, IBINOP=1 would accept the opacity table as a binary

file, which works faster, but it is less portable.

• ITEK=50, IACC=50 – inhibits both Kantorovich and Ng acceleration (that is, they would start at 50th iteration, but the total defaults number of CL iterations is 30). This option is much safer when dealing with convective models.

• TAUFIR=1.e-7,TAULAS=1.0e2 – sets the minimum and maximum Rosseland optical depth when computing the starting LTE-gray model. In fact, TAUFIR does not have to be set because 1.e-7 is the default anyway. The model can easily be computed also with the default TAULAS (3.16e2), but one would go to unnecessary large depth in the atmosphere, which is inconsequential for the bulk of atmospheric structure and emergent radiation.

• HMIX0=1 – switches on the convection, with the mixing length equal to 1 pressure scale height.

• NDCGAP=10,ICONRE=0,IDEEPC=3,CRFLIM=-10 – this was found, by some experimentation, to be the a good set of parameters for the numerical treatment of convection, namely how the convective flux and temperature are being recalculated in the global formal solution step to lead to a stable convergence of the CL iterations. For details, refer to § 7.8.

7.10.4 Cool white dwarf model in § 6.5

The content of the keyword parameter file `cwd.flag` is as follows:

```
IFRYB=1,IHYDPR=2
IPRINT=3,ITEK=40,IACC=40
TAUDIV=1.e-2,IDLST=0
HMIX0=0.6,MLTYPE=2
NDCGAP=5,ICONRE=0,IDEEPC=3,CRFLIM=-10.
IMUCON=40,ICONRS=5
```

Here, many keyword parameters are set similarly as in the previous case of a K star; here we point out only different or otherwise interesting parameters which have the following meaning:

• IFRYB=1 – sets the global iteration method to the Rybicki scheme. As pointed out in § 6.5, this scheme works much better than the standard hybrid CL/ALI scheme as it is more stable, and the convergence rate is much faster. In the present case, this setup works well even for NLTE models (file `cwdn.flag`).

• IHYDPR=2 – sets the evaluation of the hydrogen line profiles to using the Tremblay tables, which are most suitable for white dwarf models – see § 12.1.1.

• IPRINT=3 – this setup produces more output on Unit 6 (standard output), namely a table of convection parameters printed after each completed iteration of the global linearization scheme. This is useful if something goes wrong with a treatment of convection, or with the temperature correction procedures.

• ITEK=40,IACC=40 – as is prudent for models with convection, both accelerations (Ng and Kantorovich) are turned off.

• TAUDIV=0.01 – setting the coefficients of the linear combination of the differential and integral form of the energy balance equation – see § 7.4.5. The

value of 0.01, which yields accurate results (that is, a better conservation of the total flux) than the default value of 0.5, can only be set that small if the Rybicki scheme is used.

• HMIX0=0.6 – convection is switched on; the mixing length set to 0.6 pressure scale height, which is often considered as a typical value for white dwarfs.

• MLTYPE=2 – a variant of the mixing-length description, ML2, is considered. Again, it is often used for white dwarfs.

• NDCGAP=5,ICONRE=0,IDEEPC=3,CRFLIM=-10. – analogous as before.

• IMUCON=40,ICONRS=5 – additional convection parameters.

The keyword parameter file for a NLTE models, `cwdn.flag`, is very similar, the only difference is:

• ITEK=20,IACC=14 – the Ng acceleration now starts at the 14th iteration, and the Kantorovich acceleration at the 20th. As mentioned in § 6.5. one can afford to switch on the Ng acceleration because NLTE effects are not supposed to be influencing the temperature structure in any significant way. Moreover, the temperature structure, as well as the position of the convection zone, were well established in the previously computed LTE model. Although the model would converge without the Ng acceleration (the user may easily verify that by setting IACC=40), the Ng acceleration improves the convergence behavior significantly, as is clearly seen in Fig. 8.

7.10.5 Accretion disk around a white dwarf in § 6.6

In this case, the keyword parameter file `param` is simple:

```
ALPHAV=0.3
```

which sets the viscosity parameter $\alpha = 0.3$. Without setting it, α would be set to 0.1, which in fact is a typical value used for accretion disk studies. The present value of 0.3 has no special meaning; it was chosen just for the purposes of showing how to set α.

8 Starting model atmosphere

Except when computing an LTE model from scratch (i.e. LTE-gray model, by setting `LTGRAY = .TRUE.`) (for details, refer to Paper II, Chap. 4), a starting model atmosphere is needed. It is transmitted by input Unit 8, i.e. as a file with name `fort.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 atmospheres 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 a 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 (see § 8.2). Some examples were also presented in Paper I, § 5.6 and 5.7.

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

8.1 TLUSTY input model atmosphere

As mentioned earlier, the input file `fort.8` is an output file `fort.7` from a past run of TLUSTY. Its structure is as follows:

• **1st line**:

NDEPTH – number of depth points in which the initial model is given. Usually, but not necessarily, it is equal to the number of depth points, ND, considered for the current run. If it is not equal to ND, one has to interpolate the structure from the input model to the current column mass scale – see below.

NUMPAR – number of input model parameters in each depth:
= 3 (or 4 for disks) – for an LTE model (T, $n_{\rm e}$, ρ; plus z for disks);
> NLEVEL+3 (or 4 for disks) – for a NLTE model (as above, plus populations of all explicit levels of the input model).

• **Next block**:

DEPTH ($d = 1, \ldots,$NDEPTH) – depth grid for the input model, i.e. the column mass [g cm^{-2}] for all depth points. If INTRPL=0 and NDEPTH=ND, this depth grid will be used for the current model as well (DM ≡ DEPTH). If INTRPL=0 and NDEPTH ≠ ND, the program stops.

• **For each depth point**:

T – temperature, T [K]

ANE – electron density, $n_{\rm e}$ [cm^{-3}]

RHO – mass density, ρ [g cm^{-3}]

ZD – geometrical distance from the midplane [cm] – for disks only

level populations – n_i [cm^{-3}] for $i = 1, \ldots,$NLEVEL of the input model. They are needed only for a NLTE input model, but can be present for an LTE model as well, although they will be immediately recomputed. The number of input level populations does not have to be equal to the current NLEVEL; in that case the keyword ICHANG should be coded as non-zero, and the appropriate initial populations of the current levels are computed – see below.

• If INTRPL > 0. This signifies that the current depth scale is going to be different from that for the inout model (DEPTH – see above). If so, there is an additional input from unit 8, directly after the input of model parameters, which sets the new depth scale DM (i.e. the column mass in g cm^{-2}) which will be used in the current run. All the model quantities are interpolated from the initial to the new column mass grid. The interpolation is a log-log interpolation; the numerical value of INTRPL sets the order of interpolation (INTRPL=1 signifies a linear interpolation in logarithms, INTRPL=2 the quadratic one, etc.).

8.2 Change of the input level structure

The change of the explicit level structure is controlled by parameter ICHANG – see § 7.6. If this parameter is coded negative, then an 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 the necessity to start again from the scratch.

For each explicit level in the "new" level 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.
- $= 3$ – a 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

In our experience, it is usually sufficient to use MODE=1 for the "new" levels. Recall that even if this sets the LTE populations for such levels, they will be immediately recalculated to yield an (approximate) NLTE population in the first formal solution even before entering the first linearization step.

Recall that when the keyword parameter ICHANG is set to 1 (see § 7.6), one specifies the so-called "simplified change", which can be used only if (a) one leaves the structure of the input energy levels unchanged, while (b) one only adds levels of new species, which are now indexed with I=NLEVEL0+1,...,NLEVEL, where NLEVEL0 is the number of levels in the input model. Their initial level populations are set to the LTE values. In this case, no other additional input parameters are needed.

8.3 Kurucz input model atmosphere

TLUSTY also accepts Kurucz (1979, and later Kurucz CD-ROMs) models as starting models. The format of the file is the standard Kurucz output file. The Kurucz model is read if the parameter INTRPL is set to -1.

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 the end of the Kurucz model file by the parameter INTRPL followed by the values of the column mass (in 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 keyword parameter ND should be set to 63 (i.e. `ND=63`) should appear in the keyword parameter file (see § 7.4.1).

9 Output

There are several output files. We divide them into two groups as 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 11 – Mean opacities for the resulting model
- Unit 12 – b-factors (NLTE departure coefficients)
- Unit 13 – Emergent flux in all frequency points (spectral energy distribution)
- Unit 18 – Convergence log for the formal solution
- Unit 69 – Timing log

2. Auxiliary output, generated only if required (by setting the corresponding keyword parameters – see Sect. 13.8)

   - Unit 14 – Emergent (angle-dependent) specific intensities in all frequency points (at present it is implemented only in the case of Compton scattering)
   - Unit 16 – A check of the accuracy of the numerical solution of the kinetic equilibrium equation
   - 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

9.1 Basic standard output

Unit 6: Standard output.

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

The amount of output on Unit 6 depends upon input parameters. For instance, an 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 keyword parameter file.

Unit 7: Condensed model atmosphere.

This is the basic output in a machine-oriented form, i.e. without any table headers, etc. This file may serve as the input model file for another run of

TLUSTY as Unit 8, or for SYNSPEC and various interface and utility programs. Its structure is described in detail in § 8.1.

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. As mentioned in § 6.1 ,there is also an IDL routine `pconv` for plotting its contents. The individual columns have the following meaning:

1. iteration number
2. depth index (d)
3. relative change in T, i.e. $(T_d^{\rm new} - T_d^{\rm old})/T_d^{\rm new}$
4. relative change in $n_{\rm e}$, (defined analogously)
5. maximum relative change of all explicit level populations
6. maximum relative change of linearized mean intensities
7. maximum relative changes of all component of the state vector
8. index of the level population that exhibits the maximum relative change
9. index of the frequency point that exhibits the maximum relative change

Notice that if the Rybicki scheme is used, all the relative changes except that of temperature are equal to zero.

Unit 10: Performance and error log.

This file, created by several 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 dimensions against maximum allowed 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 11: Mean opacities for the resulting model.

This file is generated by subroutine `ROSSTD` in the final iteration. It is composed of ND records, each containing:

1. depth index
2. column mass m [g cm^{-2}]
3. Rosseland optical depth
4. Rosseland opacity per unit mass [cm^2 g $^{-1}$]
5. temperature T [K]
6. electron density $n_{\rm e}$ [cm^{-3}]
7. mass density ρ [g cm^{-3}]
8. numerically integrated Planck function, $\sum_i w_i B(\nu_i, T)$,
9. analytically integrated Planck function ($\pi\sigma_R T^4$),
10. Planck mean opacity [cm^2 g $^{-1}$]

This table, which shows the basic structural parameters (T, $n_{\rm e}$, ρ) as a function of the Rosseland optical depth is useful for comparisons with other models; a comparison of the two integrated Planck functions to check the accuracy of frequency coverage and integrations.

Unit 13 – Emergent flux.

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

1. frequency [s^{-1}]
2. emergent flux, precisely the first moment of the specific intensity of radiation, H_ν, at the surface, [erg cm^{-2} s^{-1}Hz^{-1}]
3. 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 200, additional quantities were printed out in this file.

Unit 18 – Convergence log of the formal solution.

Generated by subroutine `RESOLV`. The individual columns are:

1. iteration number of the linearization procedure
2. iteration number of the formal solution

3. depth index

4. maximum relative change of all populations

5. index of level for which the maximum relative change occurs.

This file is seldom used. It may be useful for diagnosing problems that may occur in the formal solution.

Unit 69: Timing.

As pointed out above, this file is produced only under Unix or Linux. The individual columns represent:

1. iteration number

2. a label for distinguishing the two parts of the given iteration step: 1 for the global formal solution part (subroutine `RESOLV`), and 2 for the linearization part 1 (subroutine `SOLVE`);

3. total elapsed time up to the given step [s]

4. time spent in the given step [s]

5. a descriptive label corresponding to the second column.

9.2 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 kinetic equilibrium equations.

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

These files are completely analogous to the 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 iteration crashed or diverged due to numerical reasons (e.g., an improper use of acceleration techniques, etc.).

Units 85 and 86 - opacities and other quantities for the continuum frequencies.

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

- = 1 – 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.
- = 2 – a more extended table with the frequency index and the value of frequency, followed by ND records for each depth that contains 5 numbers: the monochromatic optical depth, the true absorption coefficient, scattering coefficient, emission coefficient, and the mean intensity of radiation.

Units 87 and 88 - cooling rates.

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

Unit 87 contains four columns; the depth index, the total net cooling rate without an influence of scattering ($C_{\rm net}$), the total net cooling rate including scattering ($C'_{\rm net}$), and the total cooling rate (i.e., the true radiative cooling without a balancing effect of radiation heating, $C_{\rm tot}$). 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).

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

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

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

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

If IPRINP is set to a value larger than 10, an additional output is generated – Unit 88 – that contains the cooling rates separately for all explicit ions separately.

10 Basic troubleshooting

Here we describe the most common errors when running TLUSTY, and the ways to fix them. Advanced troubleshooting, and a summary of useful numerical and physical tricks, will be covered later in § 15 in Part II.

10.1 Program stops immediately

On several occasions, the program stops either immediately, or after a few seconds. There are several possible errors:

- No standard output created, and the message

  ```
  Wrong architecture
  ```

  or

  ```
  dyld: Library not loaded: /usr/local/lib/libg2c.0.dylib
  Referenced from: ...
  Reason: image not found
  Trace/BPT trap
  ```

  is generated. This indicated that the code was compiled on a different machine and the executable was accidentally copied. The fix: recompile the code on the current machine.

- Program stops with the message:

  ```
  Bus error
  ```

  Most likely, the core memory is not sufficient to run the current executable. The fix: run the PRETLUS program with the standard input for the current model, and update the `BASICS.FOR` and `ODFPAR.FOR` files accordingly, and recompile TLUSTY. If the problem persists, the core memory of the computer is not sufficient to run the code with the current input data. One has to modify the input data to make the model less demanding on the computer memory, for instance, by decreasing the number of explicit ions, levels, frequencies, depths, etc. (Obviously, a better option is to use a computer with a larger memory.)

- Program stop with a message

  ```
  Segmentation fault
  ```

  Most likely, the code was not compiled with the specification `-fno-automatic`. The fix: recompile the code with `-fno-automatic` (or `-static` for the generic Unix), and run again.

- The program runs for a short time, and generates some content to the standard output file (the header, plus possibly a few tables), and then stops. In this case inspect the standard output, in particular the end of it. The last line will most likely contain a message that a dimension of some array is larger than the maximum available dimension. For instance, the last line of the standard input may read

```
ilev.gt.mlevel          164       134
```

which means that the level index `ilev` (=164) surpassed the maximum number of explicit levels (MLEVEL=134), set up in the "INCLUDE" file BASICS.FOR (see § 2.2).

The fix: run the PRETLUS program with the same input data as the current mode, and check whether all the dimension parameters in BASICS.FOR and ODFPAR.FOR are larger than or equal to the values specified by the PRETLUS output. It is much preferable to run PRETLUS, because the above message does not mean that it is sufficient to reset MLEVEL to, say 165, because TLUSTY stopped in the first occurrence of `ilev` > MLEVEL, but had it continued it could have reached much higher values of `ilev`. In such a case, the user would have to recompile and rerun the code many times.

- Program may also stop because some file, whose need is stipulated by the input data, is missing. A message is issued to this effect. The obvious fix is to provide the needed file, or, if the file is not available, to run the code with the input parameters that do not require such a file.

10.2 Program runs, but does not converge

This is of course the most common problem, and often the most difficult to solve. There is no general recipe for fixing it. However, it is our belief that for any model, regardless how complex it may be, there is essentially always a way to converge it within the means provided by TLUSTY, but sometimes it is very difficult to find the proper way. Over the time, we have developed many strategies and procedures to help with convergence problems, but while one strategy may work perfectly in some cases, it could rather cause problems in others. Therefore, finding a good way to converge a model is sometimes a true art.

Here we will provide a guidance about possible strategies that are worth trying in difficult cases. We will consider separately several classes of models, starting with some general strategies applicable for all models.

10.2.1 General strategies

The most important part of the diagnosis of the problem is to inspect the convergence log, output file `fort.9`, preferably by plotting its contents using our IDL routine `pconv`, or, if IDL is not available, to write an analogous routine in a graphical package that is available. Sometimes it is also worthwhile to inspect the standard output, in particular for convective models.

Here we list several general symptoms, and corresponding strategies to fix the problem.

- If the relative changes, in particular the maximum change over all depths (the rightmost panels in Figs, 1, 4, 7, 8) exhibits a sudden increase in the

7th iteration while the keyword IACC that specifies the Ng acceleration is not set, thus assuming its default value IACC=7 (or if IACC is specifically set differently, and an increase of the maximum relative change occurs at the iteration number IACC), then there is a good probability that the culprit is the Ng acceleration.

The fix: increase IACC to start the Ng acceleration later, or disable it completely (by setting IACC larger than NITER).

- An analogous problems may happen if the Kantorovich acceleration is switched on too early. Again, a symptom would be that the relative changes exhibit strange increase at the iteration at which the Kantorovich scheme is set (controlled by the keyword ITEK, with the default equal to 4). This scheme usually does not cause divergences but rather only a slower convergence, but it may cause problems if a model structure changes dramatically at iteration steps after the ITEK-th iteration. For instance, the convection zone may easily change position, so the Jacobi matrix evaluated in an earlier iteration step would be inconsistent with the present atmospheric structure.

- The convergence pattern exhibits a spike, or a sudden increase, at the depth point which corresponds to TAUDIV, the point at which the coefficients of the linear combination of the integral and differential form of the radiative equilibrium equation suddenly change (called the division point). This depth is found in the standard output in the table entitled:

  ```
  id        redif          reint
  ```

  where `id` represent the depth index, `reint` and `redif` are the parameters α and β in Eq. (16) of Paper II, respectively. The division point is the depth where `redif` suddenly changes value from 0 to 1.

  A possible fix: try to change the value of keyword TAUDIV, or, perhaps much better, to set the basic mode of calculation to the Rybicki scheme (IFRYB=1). There are some other possibilities; we will mention some of them below when dealing with specific types of models.

10.2.2 LTE models without convection

Non-convective LTE models are usually the easiest to converge, but even in this case one may sometimes face problems. Here are several typical situations:

- If one faces generic convergence problems or a divergence not related to the cases described above, the first possible fix is again to set the basic mode of model calculation to the Rybicki scheme. In most cases it helps significantly.

- If there are problems even with the Rybicki scheme being set, and in particular if the relative changes are large in the upper layers, the problems

may be connected to spectral lines. In that case, try first to converge a model without any lines (as is done, for instance, in the first H-He model in § 6.2), and then to add lines. If there are still problems, one may try to converge first a model with fewer lines and consecutively adding more, lines, as explained in § 5.1.

- If the convergence pattern exhibits large changes in deep layers (possibly oscillating and increasing in absolute value), and the Rybicki scheme does not help, then the problem may be that the model is in fact convective, but the convection was not set up (HMIX0 ≤ 0). The obvious fix is to set up the convection, HMIX0 > 0.

10.2.3 LTE convective models

The first action one needs to take in the case of convergence problems with LTE convective model is to rerun the model with IPRINT=3, in which case the standard output will contain the table of interesting model quantities that enter the evaluation of the convective flux, together with the corrected temperature in the case of one or both of the correction procedures described in Paper II, Appendix B2 and here in § 7.8 are applied. One can use the test cases considered in § 6.4 and § 6.5 as a template, but if that does not work, one has to experiment with changing the individual parameters to see whether that helps. The hints how to set up some parameters (e.g., NDCGAP, IDEEPC) are given in § 7.8; the parameters ICONRE, ICONRS, and IMUCON that set the first and the last iteration step at which the correction procedures are performed have to be found by trial and error. Unfortunately, we do not know of any general recipe that would be applicable in all cases.

Interestingly, the correction procedures work best for a strong convection (where the dominant part of the flux is transported by convection), in which case the temperature gradient is close to the adiabatic gradient. Convection is more difficult to treat, and the correction procedures may not be helping, if the convection is weak but still present. But in those cases the Rybicki scheme, if not already set, may help significantly.

10.2.4 NLTE models

Again, there is no general recipe to fix the convergence problems for NLTE models. All the strategies described in § 10.2.1 and 10.2.2 are of course applicable here as well. Some additional possibilities are described below:

- One may try to increase NLAMBD, the number of global formal solutions between two consecutive iterations of the linearization scheme, setting for instance NLAMBD=4.

- If the strategy of converging first a model without lines and then adding consecutively more and more lines does not work, one can resort to set IFIXMO=1, in which case the temperature, electron density, and mass

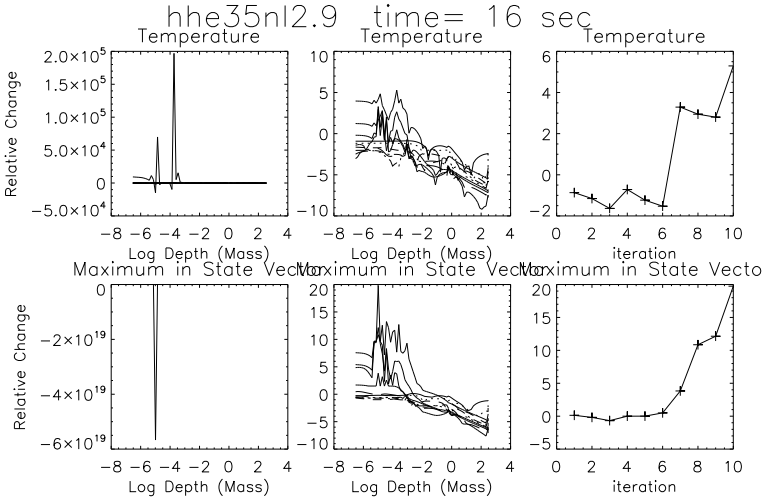

Figure 9: Convergence log for the `hhe35nl2` model.

density remain fixed to the values of the input model, and only the level populations and the radiation intensities are computed (the so-called restricted NLTE problem). This model, when converged, can be used as the input model for the subsequent run where all the state parameters are being updated. If this still does not work, one may try to first converge a model with INRE=0 (that is, keeping the temperature fixed and updating everything else), and only after that to continue to the full model.

- As demonstrated in § 6.5, it is sometimes helpful to apply the Rybicki scheme even for NLTE models. If it converges very slowly, and can still use the resulting model as a new starting model for the full NLTE solution using the default hybrid CL/ALI method.

As an example, we take a NLTE/L H-He model considered in § 6.2. First we leave the standard input data `hhe35nl.5` unchanged, but instead of starting with the NLTE/C (model `hhe35nc.7`), we take as a starting model the LTE one, `hhe35lt.7`. Although we know that it is better to start with the NLTE/C model, we take this case as an example of finding the way to converge a difficult model, or, in other words, to converge a model with inappropriately chosen initial model.

The model run is submitted as

```
cp hhe35nl.5 hhe35nl2.5
RTlusty hhe35nl2 hhe35lt
```

so that the new model files have a core name `hhe35nl2`. The convergence pattern is displayed in Fig. 9. It is seen that the maximum relative change exhibits

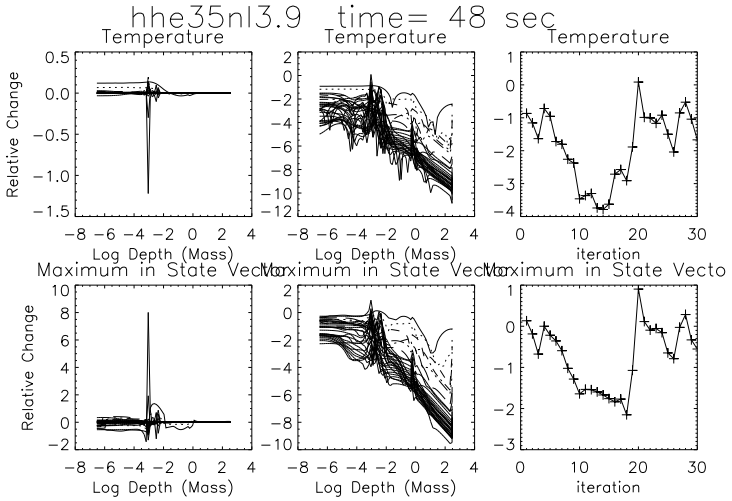

Figure 10: Convergence log for the `hhe35nl3` model.

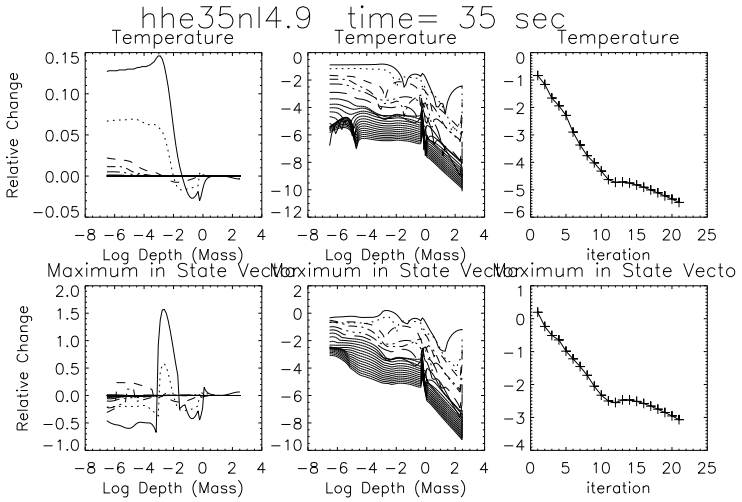

Figure 11: Convergence log for the `hhe35nl4` model.

the first large jump at the 7th iteration, which, as explained in § 10.2.1, points to the Ng acceleration as the likely source of problem. One can therefore try to disable the Ng acceleration, and to be on the safe side, also the Kantorovich acceleration. One then creates a standard input file `hhe35nl3.5`, which is identical to `hhe35nl2.5`, except the 3rd line which now specifies the name of the keyword parameter file, `'f3'`. This file contains just one record:

```
IACC=40,ITEK=40
```

which effectively disables both accelerations. The convergence pattern of this model is shown in Fig. 10. The convergence behavior is clearly improved, but the model still cannot be viewed as converged. As suggested above, one may try to increase the number of iterations of the global formal solutions. This model, called `hhe35nl4`, has the keyword parameter file, named `'f4'` which is:

```
IACC=40,ITEK=40,NLAMBD=4
```

The convergence pattern of this model is shown in Fig. 11. Indeed, the convergence is now much better. Comparing this model and the original `hhe35nl` model considered in § 6.2 reveals that both models are essentially identical, as one should expect from two converged models computed with the same physical parameters.

There are several more advanced procedures, often applicable to special types of objects. They will be discussed in Chap. 15.

Part II

In the second part of this operational manual, we describe the topics that are not absolutely necessary for a casual user of TLUSTY, in a sense that one can construct basic model atmospheres and accretion disks using information from Part I only. However, the material presented in Part II is quite important for a dedicated user. It provides a more detailed understanding of the employed numerical procedures, the treatment of input atomic data, the calculation of specific models, as well as the description of additional flags that help cope with convergence problems.

11 Input files for individual model atoms

Each explicit ion has an individual file which contains information about three or four basic types of atomic data (the fourth type is only required in the Opacity Sampling 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, such as the oscillator strengths, line broadening parameters, a mode of evaluation of the collisionakl excitation rates, etc.).
4. Energy bands for setting up superlevels of iron-peak elements (only required in the Opacity Sampling mode)

The overall 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 in the standard input (unit 5). In fact, such a library is available through the TLUSTY website.[2]

Moreover, there is an IDL–based program called MODION, written by F. Varosi (NASA/GSFC), which is designed to construct the individual atomic data 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 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.

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

```
****** Levels
```

[2] `http://tlusty.oca.eu`

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. This is followed, if applicable, by

```
****** Energy bands
```

followed by limits for energy bands for superlevels, without any comment line.

We will now describe the basic blocks of the atomic data file in detail.

11.1 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. As mentioned in Paper II, § 3.6, 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);

(ii) a merged level, which is a superlevel composed of all merged Rydberg, partially dissolved, states of an ion. The level parameters, such as its statistical weight and a mean energy are considered as depth-dependent, due to a depth-dependence of the occupation probabilities that 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}). The atomic data files stored in the TLUSTY website express the ionization energy as frequency; this has an advantage that the user can immediately recognize which continuum jump in the predicted emergent spectrum corresponds to which ion.

- if = 0 – the program assigns the hydrogenic value, $E = Z^2 E_H / n^2$, where Z is the charge of the next ion, E_H the ionization energy of hydrogen ($E_H = 3.28805 \times 10^{15}$ in the frequency units), and n is the principal quantum number. Here it is assumed that the principal quantum number is the order number of level within the corresponding ion.

G – statistical weight;

- if = 0 – the program assigns the hydrogenic statistical weight, $g = 2n^2$.

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 in outputs, but may also be used as an identifier in the case of using the pre-tabulated photoionization cross section data.

IFWOP – a mode of the treatment of level dissolution (see Paper II, § 2.6):

- $= 0$ – 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 using a generalized occupation probability (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 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 – mode of treating the linearization of the level population There were several options, which all are more or less outdated. The only practical use of parameter IMODL is to set up the *level groups*.

- $= 0$ – the level is linearized individually (i.e., it forms its own group);
- < -100 – the given level is a member of *level group* – see Paper II, § 3.7. A group is composed 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.

11.2 Parameters for bound–free transitions

The structure is as follows. Each transition which is 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 is 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 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 the dissolved part of a corresponding spectral series converging to the given edge – see Paper II, § 2.6. 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 (the so-called cutoff frequency).

IBF≡IFANCY – a mode of evaluation of the photoionization cross sections. All cross sections are in cm^{-2}.

- for `IBF` $= 0$ – simplified hydrogenic (Gaunt factor set to 1)
  $\sigma(\nu) = 2.815 \times 10^{-29} Z^4 \nu^{-3} n^{-5}$
- for `IBF` $= 1$ – exact hydrogenic,
  $\sigma(\nu) = 2.815 \times 10^{-29} Z^4 \nu^{-3} n^{-5} g^{\mathrm{bf}}(n, \nu/Z^2)$
- for `IBF` $= 2$ – Peach (1967) formula (obsolete)
  $\sigma(\nu) = \alpha[\beta x^s + (1-\beta) x^{s+1}] \times 10^{-18}$
- for `IBF` $= 3$ – modified Peach formula after Henry (1970) – obsolete
  $\sigma(\nu) = \alpha[\Gamma x^s + (\beta - 2\Gamma) x^{s+1} + (1 + \Gamma - \beta) x^{s+2}] \times 10^{-18}$
- for `IBF` $= 4$ – Butler (1990) fit formula of the form,
  $\sigma(\nu) = \exp[s + \alpha \log x + \beta \log^2 x]$

where $x = \nu_0/\nu$, s=`S0`, α=`ALF`, β=`BET`, and Γ=`GAM`. For the appropriate options they are given in the immediately following record. Further, n is the principal quantum number, and Z the effective charge (=1 for neutrals, 2 for once ionized, etc.), and ν_0 the threshold frequency.

- for `IBF` $= 5$ – cross section from Verner & Yakovlev (1995) tables
- for `IBF` $= 7$ – hydrogenic cross section with the Gaunt factors from Klaus Werner (priv. comm.)
- for `IBF` $= 9$ – Opacity Project data stored in a special file, named RBF.DAT (obsolete option)
- for `IBF` $= 11$ – Opacity Project cross section for He I singlet levels with Fernley et al. (1987) cubic fits
- for `IBF` $= 13$ – analogous for He I triplet levels
- for `IBF` $= 21$ – Cross section for ground state of He I from Koester (1985) fit

For the last three options (IBF = 11, 13, 21), the data are hardwired in the code, so no additional input is needed.

- for IBF between 50 and 99 – special cross section for a superlevel, precalculated. IBF then indicates the input unit number from which the data are read.
- for IBF > 100 – Opacity Project (OP) data, immediately following the given record. There are IBF−100 data points. This is the most common option for all the transitions for which OP data are available.
- for IBF < 0 – non-standard expression, given by a user supplied addition to the subroutine SPSIGK. This option is practically obsolete, but for directions of its use, see § 14.1.

There is one special value of IBF, namely

- for IBF = 15 – which indicates that the rest of the input file has a different form adopted for treating ions for which the inner-shell ionization is taken into account, called "X-file". The structure of this file is explained in detail in § 11.7.

ICOL – mode of evaluation of the collisional rate

- for ICOL = 0 – standard formulae, different for different species:
  – for H, He I, and He II expressions from Mihalas et al;. (1975),
  – for other species by the so-called Seaton formula
  $$\Omega = 1.55 \times 10^{13} T^{-1/2} U_0^{-1} \exp(-U_0) \sigma_0 \bar{g},$$
  where $U_0 = h\nu_0/kT$, and $\bar{g} = 0.1$ for neutral atoms, $\bar{g} = 0.2$ for singly ionized atoms, and $\bar{g} = 0.3$ otherwise. σ_0 it the photoionzation cross section at the threshold. Quantity $\bar{g}\sigma_0$ is given by the input parameter OSC0 – see below,
- for ICOL = 1 – so-called Allen formula:
  $\Omega = c_0 T^{-3/2} U_0^{-2} \exp(-U_0)$,
- for ICOL = 2 : $\Omega = 5.465 \times 10^{-11} c_0 T^{1/2} \exp(-U_0)$,
- for ICOL = 3 : $\Omega = 5.465 \times 10^{-11} c_0 T^{1/2} (1 + U_0) \exp(-U_0)$
  where in the three above options c_0 is given by OSC0,
- for ICOL = 4 – collisional rate evaluated by subroutine cion adapted from program XSTAR by T. Kallman. This is used only in X-files.
- for ICOL = 5 – collisional rate evaluated by subroutine irc, adapted from program XSTAR by T. Kallman. Also used only for X-files.
- for ICOL = 10 – radiative charge transfer ionization with protons is added to the ordinary collisional ionization rate. It can be used only for the ground states of neutral atoms. This represents an additional means of including the charge transfer reaction, in this case selectively for a particular atom. As described in § 12.3.2, one can also switch on this reaction for all neutral atoms by setting the keyword parameter IFCHTR to a non-zero value.

- for `ICOL` = 99 – collisional rate is set to zero, $\Omega = 0$. Again, used only in X-files for Auger processes.
- for `ICOL` < 0 – non-standard expression, given by a user–supplied procedure (CSPEC). Practically obsolete, but for its use see § 14.3.

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 – collision parameter entering the above expressions, i.e. $\bar{g}\sigma_0$ in the case of Seaton formula (ICOL=0); or c_0 for ICOL=1, 2, 3.

CPARAM – dummy parameter for bound-free transitions.

Additional input parameters for continuum transitions

In most cases, there is one or more additional input records for continuum transition, which depend on the 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. the 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; i.e., the cutoff frequency for the pseudo-continuum opacity (see Paper II, § 2.6). In the case of the Lyman and Balmer continuum of hydrogen, it may be overwritten through the keyword parameters CUTLYM and CUTBAL - see § 12.4.

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

S0, ALF, BET, GAM – parameters for the evaluation of the photoionization cross section in the Peach, Henry, and Butler form – see above.

(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.

11.3 Parameters for bound-bound transitions

The structure is analogous to that for the bound-free transitions, § 11.2. Each transition which is 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 the radiative rates in the transition.

- $= 0$ – detailed radiative balance (ie. radiative rates are set to zero but collisional rates are evaluated);
- > 0 – primarily linearized transition;
- < 0 – primarily ALI transition;
- $= 1$ or -1 – an "ordinary" line (i.e., any line represented by a symmetric profile (Doppler, Voigt, or special profiles for hydrogenic lines - see below)
- $= 2$ or -2 – a "merged" line, 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 corresponding Opacity Distribution Function is calculated by TLUSTY. This option is typically used for H and He II.
- $= 3$ or -3 – a superline, treated either, (i) in the Opacity Sampling mode (a standard option), in which TLUSTY computes the detailed cross sections from the basic atomic data, usually given by Kurucz atomic data files, or, (ii) In the Opacity Distribution Function (ODF) mode, in which case the ODF is calculated by a separate program, and is communicated to TLUSTY by means of two additional input files As mentioned above, this option is now obsolete.

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

- $= 0$ – Doppler profile;
- $= 1$ or -1 – Voigt profile;
- $= 2$ or -2 – approximate Stark (+ Doppler) profile for hydrogenic lines after Hubeny et al. (1994);
- $= 3$ or -3 – hydrogen line profiles given by Lemke's tables.

• $= 4$ or -4 – hydrogen line profiles given by Tremblay's tables.
However, if the keyword parameter IHYDPR is set to a non-zero value, the Lemke or Tremblay 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. For details, refer to § 12.1.1.
• ≥ 10 – non-standard expression, given by a user-supplied subroutine (PROFSP);
• > 0 – the absorption profile at the farthermost frequency point(s) from the line center is(are) taken to be 0;
• < 0 – the absorption profile at the farthermost frequency point(s) is(are) evaluated exactly.

ICOL - mode of evaluating the collisional rates. The meaning of ICOL is different for H and He, and for other species.

Specifically for H and He:

- for `ICOL` $= 0$ – standard approximate expression taken from Mihalas et al. (1975).

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

- for `ICOL` $= 1$, 2, or 3 – much more accurate by Berrington & Kingston (1987) rates, subroutine written by D.G.Hummer (COLLHE). This procedure can be used only for transitions between states with $n = 1, \ldots 4$.
- for `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.
- for `ICOL` $= 2$ – means that a given transition is a transition between a non-averaged ls lower state and an averaged upper state.
- for `ICOL` $= 3$ – means that a given transition is a transition between two averaged states.

For species other than H or He:

- for `ICOL` $= 0$ – simplified van Regemorter (1962) formula $\Omega = 19.7363\, f_{ij} T^{-3/2} U_0^{-1} \exp(-U_0) \max\left[\bar{g}, 0.276 \exp(U_0) E_1(U_0)\right]$, with $\bar{g} = 0.25$
- for `ICOL` $= 1$: proper van Regermorter formula; the same as above, but now $\bar{g}$ is an input parameter (`CPAR`). $\bar{g}$ 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` $= 2$: $\Omega = 5.465 \times 10^{-11} f_{ij} c_0 T^{1/2} \exp(-U_0)$,
- for `ICOL` $= 3$: $\Omega = 5.465 \times 10^{-11} f_{ij} c_0 T^{1/2} (1 + U_0) \exp(-U_0)$,

- for `ICOL` = 4 : Eissner-Seaton (1972) formula:
  $\Omega = 8.631 \times 10^{-6} g_i^{-1} T^{-1/2} \exp(-U_0) c_0$.
  In the three above options c_0 is given by input parameter `CPARAM` – see below
- for `ICOL` = 9 : represents the collision rate for a superline, computed by summing collision strengths for the individual components.
- for `ICOL` = -1 :Van Regemorter formula for neutral atoms,
  $\Omega = 19.7363\, f_{ij}\, T^{-3/2}\, U_0^{-1} \exp(-U_0)\, \Gamma(U_0)$, where
  $\Gamma(U_0) = 0.276 \exp(U_0)\, E_1(U_0)$, for $U_0 \leq 14$, and
  $\Gamma(U_0) = 0.066\, U_0^{-1/2}\, (1 + 1.5 U_0)$, for $U_0 > 14$

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.

Generally, for any species,

- for `ICOL` < 0 – non-standard expression, given by a user–supplied addition to the subroutine CSPEC. This option is practically obsolete, but for its use see § 14.3. The value of ICOL= -1 is already used for the Van Regemorter formula for neutral atoms - see above.

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

CPARAM – collision parameter, i.e. quantity $\bar{g}$ for ICOL=1, or c_0 for ICOL= 2, 3, 4.

Additional input parameters for line transitions

In most cases, there is one or more additional input records for the line transition, which depends on the 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, to avoid a spurious overlap of a normal line and a superline represented by an ODF. Again, it is obsolete in the Opacity Sampling mode.

(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. This option is cumbersome to use, and is generally obsolete.

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

XMAX – the maximum frequency extent of the line, in units of fiducial Doppler width, defined as the Doppler width for the given species evaluated at $T =$ TSTD, and the standard microturbulent velocity VTB– see below:
- $= 0$ – 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. But see the note below.
- < 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 $2 \times \mathrm{NF} - 1$.

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

(3) If a Voigt profile is assumed, i.e., if abs(IFANCY) = 1, an additional input record is required which specifies an evaluation of the relevant damping parameter:

GAMR – a natural broadening indicator:
- > 0 – has the meaning of natural damping parameter;

- $= 0$ – classical natural damping assumed $\Gamma = 2.4734 \times 10^{-8}\,\nu_0^2$;
- < 0 – natural damping is given by a non-standard, user supplied expression in the subroutine GAMSP – see § 14.2,

STARK1 – Stark broadening indicator:
- $= 0$ – Stark broadening is neglected;
- < 0 – scaled classical expression, i.e. $\Gamma = -\texttt{STARK1} \times \Gamma^{\rm clas}$, where $\Gamma^{\rm clas} = 10^{-8}\, n_{\rm eff}^{5/2}\, n_{\rm e}$, where $n_{\rm eff}$ is the effective quantum number of the upper level, $n_{\rm eff} \equiv Z_I^2 [E_H/(E_I - E_j)]^{1/2}$ with the excitation energy E_j and the ionization energy E_I, Z_I is the effective charge ($Z_I = 1$ for neutrals) of the ion I, E_H is the ionization energy of hydrogen, and $n_{\rm e}$ is the electron density.
- > 0 – Stark broadening given by $n_{\rm e}\,(\texttt{STARK1} \times T^{\texttt{STARK2}} + \texttt{STARK3})$, where `STARK2, STARK3` are the input parameters

STARK2, STARK3 – see above

VDWH – Van der Waals broadening indicator:
- ≤ 0 – Van der Waals broadening is neglected;
- > 0 – a scaled classical expression (see Paper I, Appendix A).

(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, . . . , **4), XDO(**1, . . . , 3**)** – the parameters which have the following meaning: The superline is represented by four frequency intervals. Going away from the peak of the corresponding Opacity Distribution Function, 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 taken here as that corresponding to the effective temperature.

11.4 Energy bands for superlevels

Finally, for data files of iron-peak elements one must provide the limits of energy bands used to build the superlevels, first for even-parity levels, then for odd-parity levels. This is required only in the Opacity Sampling mode where TLUSTY reads the detailed lists of individual energy levels from the Kurucz files and constructs the superlevels. This list of energy bands must be consistent with the level data given at the top of the file. The structure of the input is as follows:

NEVKU – number of even superlevels

and then NEVKU records for i=1,. . . ,NEVKU

XEV(i) – upper energy limit for the I-th even superlevel [cm^{-1}];

and analogously for odd superlevels

NODKU – number of odd superlevels

and then NODKU records for i=1,...,NODKU

XOD(i) – upper energy limit for the i-th odd superlevel [cm^{-1}].

11.5 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. A "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
```

As an example of level data for other species, let us take first 10 levels of C IV,

```
****** Levels
 1.55945583E+16      2.    2  'C IV 2Se 1'  0   0.   0
 1.36613760E+16      2.    2  'C IV 2Po 1'  0   0.   0
 1.36581470E+16      4.    2  'C IV 2Po 1'  0   0.   0
 6.51537202E+15      2.    3  'C IV 2Se 2'  0   0.  -104
 5.99906956E+15      6.    3  'C IV 2Po 2'  0   0.  -104
 5.85471942E+15     10.    3  'C IV 2De 1'  0   0.  -104
 3.56244314E+15      2.    4  'C IV 2Se 3'  0   0.  -104
 3.35343089E+15      6.    4  'C IV 2Po 3'  0   0.  -104
 3.29290270E+15     10.    4  'C IV 2De 2'  0   0.  -104
 3.29005464E+15     14.    4  'C IV 2Fo 1'  0   0.  -104
```

Notice that both levels of the ^2P doublet (levels No. 2 and 3) are treated separately; therefore the two components of the resonance doublet at 1548 and 1551 Å are treated as individual lines. This example also illustrates setting level groups. The first three levels are treated individually, while the higher states are lumped into one group.

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

```
****** Continuum transitions
 1 10  5  1  0  1  6  0.  0.     ! Lyman cont.+ pseudocontinuum
 2.60D15                         ! Lyman pseudocontinuum cutoff
```

The 6-th and 7-th entry, IFRQ0 and IFRQ1, signify that the 1st through 6th frequency points in the Lyman continuum (the points immediately blue-ward 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 provided by a specification for the =bound-free transition from the ground state of C IV, viz.

```
****** Continuum transitions
   1  26   1    116      0      0      0   1.922E-19   0.000E+00
 -0.0149  0.0110  0.1338  0.2761  0.3795  0.5541  0.7093  0.7545
  0.7610  0.7675  0.7739  0.7804  0.7998  0.9744  1.1619  1.3246
 -0.1726 -0.2005 -0.4114 -0.6842 -0.8897 -1.2472 -1.5886 -0.5243
 -0.4333 -0.3678 -0.3427 -0.3320 -0.3668 -0.8011 -1.2988 -1.7537
```

which shows how to use a fit point representation of the Opacity Project photoionization data. In this case, there are 16 points (IFANCY=116), 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 $\bar{g}\sigma_0 = 1.922 \times 10^{-19}$ – the 8th entry. Since this model atom for C IV has 25 discrete levels, the index of the upper level of the transition – the ground state of the next ion – is 26.

Line transitions

The hydrogen Lα line is specified, for instance, by

```
 1  2 -1    2  0 26 28  0.  0.    ! H I Lyman lines
  T 3 27 1022. 0.
```

In this case, the line frequencies are predominantly taken in the ALI mode (MODE=−1), but points 26 – 28 are set to a different treatment, i.e. are linearized. The line is taken with a depth-dependent (LCOMP=T), with approximate Stark + Doppler profile (IFANCY=2). The line is assumed to extend to 1022 fiducial Doppler widths. The number of frequency points is set to 27 (NF=27), but we assume the standard value of the line-overlap mode switch IOVER=1, in which case the line is automatically taken with a full profile (extending to both sides from the line core), with the actual number of frequency

points being therefore $2 \times 27 - 1 = 53$. The line frequencies are taken with ALI except the three frequency points, 26 – 28, around the center which are linearized.

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, nor 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 the respective photoionization rates.

Another example is the beginning of the block of line transitions in the C IV model atom; here we show the transitions from the ground state (1) to the first 10 levels,

```
  1   2  -1   1   1      0      0   0.952E-01   7.000E-01
T  3   23 700.  0.
2.6E+8  7.9E-7   0.  0.  0.
  1   3  -1   1   1      0      0   1.900E-01   7.000E-01
T  3   23 700.  0.
2.6E+8  7.9E-7   0.  0.  0.
  1   4   0   0   4      0      0   0.000E+00   5.000E-02
  1   5  -1   1   1      0      0   2.030E-01   2.000E-01
T  3   21 500.  0.
4.6E+9  3.1E-6   0.  0.  0.
  1   6   0   0   4      0      0   0.000E+00   5.000E-02
  1   7   0   0   4      0      0   0.000E+00   5.000E-02
  1   8  -1   1   1      0      0   6.100E-02   2.000E-01
T  3   15 100.  0.
2.9E+9  9.4E-6   0.  0.  0.
  1   9   0   0   4      0      0   0.000E+00   5.000E-02
  1  10   0   0   4      0      0   0.000E+00   5.000E-02
```

Here, only the transitions from level 1 to levels 2, 3, and 8, are dipole allowed; the rest are dipole forbidden. The allowed transitions are treated with Voigt profile (IFANCY=1); one has therefore three record for these lines; the last of them specifies the damping parameters, in this case for the radiative and Stark broadening.

11.6 Optional, non-standard parameters

Unlike in the previous part of this chapter, the following parameters are communicated to the program through the *standard input file*. If the parameter

NONSTD of the standard input (see § 4.2) is coded as positive, the program reads an additional record with the following four parameters. These are included for historical reasons and for possible comparisons with results from the older codes (such as that of Mihalas et al. 1975), otherwise they are obsolete and hardly ever used for real calculations.

IUPSUM – mode of evaluation of the total population of higher, non-explicit, LTE energy levels of the ion – the so-called upper sum (see Paper II, § 2.3):
$= 0$ – calculated by means of the partition function
> 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. The absolute value of IUPSUM specifies the main quantum number of the highest hydrogenic level considered.
DEFAULT: IUPSUM$=-100$ for H; and $=0$ for other species.

ICUP – mode of considering a "modified collisional ionization rate", i.e., that allowing for collisional excitation into, and collisional de-excitation 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, i.e. 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

11.7 X-files: Atomic data files for inner-shell ionization

When inner-shell ionization is taken into account, the system of input explained in the previous section cannot be used, because (i) one deals with a different form of cross sections, and, most importantly, (ii) when reading data for one ion the indices of energy levels are set for this particular ion, but the actual

index of the level where an atom ends after an inner-shell ionization (two or more ionization stages higher) is not yet known.

Therefore, there is a different format of such atomic input files. Also, the number of explicit energy levels of all ions treated this way is limited to 1, i.e., these ions are treated as 1-level ions. The atoms and ions for which one does not require a consideration of inner-shell ionization are treated in the ordinary way, with as many explicit levels as desired. Obviously, the latter approach is used for H and He, but can be used for other species as well. The atomic data files for ions with inner-shell ionization, which is important in particular in the X-ray region, are called here "X-files."

The first four lines of an X-file is analogous to the ordinary atomic data file, Here is an example for C III:

```
****** Levels
 1.15792157E+16      1.    2  'c3   1Se 1'  0   0.  0
****** Continuum transitions
   1 1004 1 15 4 0 0 0.000E+00 0.000E+00
```

Data for the one (ground) level is exactly as explained before. It is followed by a label "`****** Continuum transitions`", followed by the record containing the introductory data and flags for the first possible ionization from this level.The meaning of the individual entries is similar to that in the ordinary files. Here is a detailed explanation:

II – relative index of the lower level as before, but it is always 1 because one deals with 1-level ions only.

JJ – here, instead of the relative index of the upper level, this number has to be set to be larger than 1000, and JJ-1000 represents the core charge of the ion in which the process ends. In this particular case, it ends in C IV (or C^{+3}, with a core charge 4 and the actual charge 3). In this particular case, one has in fact a regular photoionization, but which is treated analogously, and using analogous fitting formulae, as for inner-shell photoionizations (see below).

MODE – the number has to be set to 1, which indicates that the process is being treated as an explicit transition.

IBF – has to be set to 15, which tells the program that the rest of the file is an X-file, with a different meaning of the subsequent entries.

ICOL – a special flag for the corresponding collisional rate It has to be set to either 4 or 99

- = 4 – collisional ionization rate evaluated by subroutine `cion` adapted from program XSTAR by T. Kallman. The necessary fitting data are hardwired in TLUSTY, so no additional data are necessary.
- = 99 – collisional rate is set to zero.

the next three entries – all zeros, have no meaning in an X-file.

Then, there are five lines of input, again for example for the same C III X-file,

```
4.789E+01
 4 3 2
  1.208
 2
  0.0047
```

which have the following meaning
E – the threshold energy of the transition (in eV)
NMAX, IZX, NSH
S
NA
DX
which is followed by NA numbers $b_j, j = 1, \ldots, NA$, and NA groups of 11 numbers $a_{ij}, i = 1, \ldots, 11; j = 1, \ldots, NA$. In the present case, this block looks is:

```
6.000e-02
3.000e+02
-5.258768e+01
-1.632927e+02
-1.728917e+02
-8.205509e+01
-1.465739e+01
0.
0.
0.
0.
0.
0.
+3.220718e+00
-2.712337e+00
-2.975667e-01
+8.581632e-02
-3.513528e-02
+8.835004e-03
0.
0.
0.
0.
0.
```

Here, a and b, together with the rest of above input parameters, are the fitting coefficients for evaluating the corresponding photoionization cross section, using the same approach as in the XSTAR program by T. Kallman (subroutine `bkhsgo` there), adapted to TLUSTY by O. Blaes.

The next record is:

```
1 1005 1 15 99 0 0 0.000E+00 0.000E+00
```

that specifies data for the true inner-shell ionization process that leaves the C^{+2} ion in the ground state of C^{+4}. This entry is then followed by an analogous set of entries to specify the corresponding photoionization cross sections.

We stress that an X-file for a given ion contains the data for all transitions that go from this ion to a higher ion.

12 Keywords for additional/non-standard physical processes

In this chapter we describe the keyword parameters that switch on, or provide additional parameters for, additional physical processes that are not considered by default. For some specific applications, these may actually be quite important; for instance for white dwarfs, cool stars, very hot stars, or accretion disks, etc. The users who intend to use TLUSTY for such applications are encouraged to study the appropriate parts of this chapter in detail.

12.1 Hydrogen line profiles

There are two different types of refinements for the hydrogen line broadening: (i) using detailed hydrogen Stark broadening tables constructed by Lemke (1997) or Tremblay & Bergeron (2009)—hereafter referred to as Tremblay's tables; and (ii) considering the quasi-molecular satellites of Lyman α, β, γ, and Hα. We shall describe them below.

12.1.1 Special Stark broadening tables

IHYDPR – a mode of treatment of the hydrogen line broadening. This keyword can be used to set the treatment of all Lyman and Balmer lines globally, and its action overwrites the setup specified in the atomic data file through the parameter IFANCY – see § 11.3.

- = 0 – hydrogen line broadening is treated as before (an approximate Stark broadening after Hubeny, Hummer, & Lanz 1994), or whichever treatment was specified individually through parameter IFANCY in the atomic data file;
- = 1 – hydrogen line broadening is computed using Lemke's tables, for all Lyman and Balmer lines with a principal quantum number of the upper level ≤ 10, that are treated explicitly. The file `lemke.dat` has to be present in, or linked to, the current directory. The table contains data for higher lines as well, but these are not used because they turned out to be incorrect.
- = 2 – hydrogen line broadening of all Lyman and Balmer lines is computed using Tremblay's tables. The file `tremblay.dat` has to be present in, or linked to, the current directory.

DEFAULT: IHYDPR=0

12.1.2 Hydrogen quasi-molecular opacities

An interaction of a radiating hydrogen atom with neighboring protons is usually described through the pressure broadening of hydrogen lines. However, an interaction with a very close proton leads to the formation of a transient H_2^+ molecule, and the optical properties have to be described through the wave functions of this molecule. This gives rise to a number of discrete features, called quasi-molecular satellites of hydrogen lines, usually of Lyman or Balmer, lines. This effect is important for high densities, so it may play an important role in the atmospheres of white dwarfs; in some cases also in the atmospheres of extremely metal-poor stars.

The process is included in TLUSTY by means of computing the relevant cross sections using the tables by Allard & Koester (1992). The cross sections were calculated for a single, characteristic, temperature. One can also use newer, temperature-dependent cross sections supplied by N. Allard (private comm.).

When including the quasi-molecular satellites, they are treated as part of the corresponding hydrogen line profile. The full profile is computed as specified by the keyword parameter IHYDPR (§ 12.1.1). Half of the cross section, corresponding to the broadening by electrons is kept, while the other half is replaced by the data for quasi-molecular satellites that correspond to the broadening by protons (the tables extend to the whole extent of the profile, not just over the satellite features themselves).

The present version of TLUSTY deals with satellites of Lyman α, β, γ, and Balmer α, which are the most important lines. Here is a description of the corresponding keyword parameters:

IQUASI – a 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 some or all additional parameters NQUALP, NQUBET, NQUGAM, and NQUBAL (see below).

DEFAULT: IQUASI=0

NQUALP – a non-zero absolute value specifies that the satellites of Lα are taken into account. Unlike previous versions the actual number of the parameter is inconsequential.
- > 0 – standard, temperature-independent cross section. The corresponding file `laquasi.dat` has to be present in, or linked to, the current directory.
- < 0 – temperature-dependent cross section. This option requires a different table than that used in the previous option, which is not a part of the standard distribution of TLUSTY.

DEFAULT: NQUALP=0

NQUBET – an analogous flag for the Lβ satellites.
- > 0 – standard, temperature-independent cross section. The corresponding file `lbquasi.dat` has to be present in, or linked to, the current

directory.
• < 0 – temperature-dependent cross section.
DEFAULT: NQUBET=0

NQUGAM – an analogous flag for the Lγ satellites.
• > 0 – standard, temperature-independent cross section. The corresponding file `lgquasi.dat` has to be present in, or linked to, the current directory.
• < 0 – temperature-dependent cross section.
DEFAULT: NQUGAM=0

NQUBAL – an analogous flag for the Hα satellites.
• > 0 – standard, temperature-independent, cross section. The corresponding file `lhquasi.dat` has to be present in, or linked to, the current directory.
• < 0 – temperature-dependent cross section.
DEFAULT: NQUBAL=0

TQMPRF – takes effect only if one considers temperature-dependent cross section(s), where, if set to a non-zero value, TQMPRF specifies the temperature for which the cross section will be taken, so that the profile will be temperature-independent after all. It can be used for testing purposes to examine the temperature dependence of the profiles.
DEFAULT: TQMPRF=0.

12.2 Additional opacities

Some additional opacities are already hardwired in TLUSTY, so that no additional input files are necessary to describe them. Some may be switched on by setting an appropriate keyword parameter, and/or by providing a corresponding additional input file containing their tabular values.

To the first category opacities contains the hydrogen Rayleigh scattering, and the H^- opacity, although these may also be treated differently, and the H_2^+ opacity. The second category contains hydrogen quasi-molecular opacities, described above, and the Collision-Induced Absorption (CIA) opacities. We shall describe them below.

12.2.1 Rayleigh scattering

The cross section is treated either through an analytic expression (for hydrogen), or through a corresponding table that may contain contributions from many species. The former option can be used with both the standard mode (an evaluation of opacities on the fly), or with the opacity table mode, while the latter is used only in conjunction with the opacity table mode (IOPTAB < 0).

The analytical expression for hydrogen is from Kurucz (1970):

$$\sigma(\nu) = 5.799 \times 10^{-13} x^{-4} + 1.422 \times 10^{-6} x^{-6} + 2.784 x^{-8}, \qquad (3)$$

where $x = 2.997925 \times 10^{18} / \min(\nu, 2.922 \times 10^{15})$.

IRSCT – a switch for including Rayleigh scattering on hydrogen;
- $= 0$ – Rayleigh scattering is neglected.
- > 0 – Rayleigh scattering is included, using eq. (3)

DEFAULT: IRSCT=0

IFRAYL – a switch for a treatment of Rayleigh scattering in the case of using the opacity table (IOPTAB < 0);
- < 0 – the scattering coefficient, possibly for many species, is given by the special table called `rayleigh.tab` which has to be given in the same grid of temperatures, densities, and frequencies as the global opacity table `absopac.dat`;
- > 0 – the scattering coefficient, only on hydrogen, is still evaluated by an analytical formula using eq. (3).
- $= 0$ – Rayleigh scattering is neglected.

DEFAULT: IFRAYL=0

12.2.2 Hardwired optional H and He opacities

The following keyword parameters, if set to a non-zero value, switch on the individual opacity sources described below. If switched on, their evaluation does not require any additional input data.

IOPHMI – a switch for including the H^- opacity (both bound-free and free-free), assuming LTE. Note that H^- can be considered as one of the explicit ions, then the opacity is calculated automatically (and moreover in NLTE if such a model is being calculated). In this case one must code IOPHMI=0 in order not to include the H^- opacity twice. In both cases, selecting H^- as a one-level separate ion, or using this option, IOPHMI > 0, the bound-free as well as free-free opacity due to H^- is evaluated using the table (for bound-free) or an analytic expression (for free-free) from Kurucz (1970).
DEFAULT: IOPHMI=0

IOPH2P – a switch for considering the H_2^+ opacity, bound bound-free and free-free, using the analytic expression from Kurucz (1970).
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 the highest level considered explicitly and an averaged level corresponding to the principal quantum number equal to IOPHE1 (after Mihalas et al. 1975). Outdated; 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 the highest level considered explicitly and an averaged level corresponding to the principal quantum number equal to IOPHE2 (again after Mihalas et al. 1975). Outdated; included for historical reasons only.
DEFAULT: IOPHE2=0

12.2.3 CIA opacities

The Collision-Induced Opacity (CIA) for H_2 – H_2 interactions, using data from Borysow & Frommhold (1990) can be included by setting the keyword parameter IFCIA. In this case, one needs an additional file `CIA-H2H2.Yi`. The corresponding subroutine was written by M. Montgomery.

IFCIA – switch for including the CIA opacity;
- $= 0$ – the CIA opacity is neglected;
- > 0 – the CIA opacity is included.

DEFAULT: IFCIA=0

12.3 Collisions

Although the evaluation of collisional rates is controlled by the corresponding parameters in the atomic data files (see § 11.2 and § 11.3), TLUSTY offers several keyword parameters that are designed to set up a modification of such an evaluation for a whole group of transitions without the necessity to modify the standard atomic data files.

12.3.1 Modified electron collisional rates for hydrogen

ICOLHN – a switch for setting up the default calculation of the hydrogen collisional excitation rates. We stress that setting this parameter to 1 or 2 will overwrite the mode of evaluation of collisional rates specified by input parameter ICOL (coded in the input atomic data file – see § 11.3).
- $= 0$ – hydrogen collisional excitation rates are evaluated according to the values of ICOL.
- $= 1$ – hydrogen collisional excitation rates are evaluated using the data by Przybilla & Butler (2004) (for transitions with the upper level up to $n = 7$);
- $= 2$ – hydrogen collisional excitation rates are evaluated using the data by Giovanardi et al. (1987) (for transitions with the upper level up to $n = 15$).

DEFAULT: ICOLHN=1

12.3.2 Charge transfer reactions

IFCHTR – a global switch indicating that all the charge transfer reactions of neutral or ionized atoms (with atomic numbers 2 to 30) with hydrogen are switched on. The charge transfer reaction is treated as a 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 (1996). The corresponding subroutine was written by C. Allende-Prieto. One can also set up charge transfer for individual species separately by appropriately modifying parameter ICOL (see § 11.2).

• = 0 – charge transfer is not set globally; the process can be switched on for individual ions through ICOL

• ≠ 0 – charge transfer is set globally for all species with atomic number between 2 and 30 (He to Zn). In this case, charge transfer reactions are considered up to IFCHTR-1 times ionized atoms; that is IFCHTR=1 means that the charge transfer reactions are switched on for neutral atoms only, IFCHTR=2 switches charge transfer for neutrals and once-ionized atoms, etc.

DEFAULT: IFCHTR=0

12.3.3 Dielectronic recombination

As explained in Paper II, § 2.5, dielectronic recombination is included automatically if the corresponding photoionization cross section is included with all the resonances.

If the photoionization cross section is treated as a smooth function of frequency, there is still a possibility to take dielectronic recombination into account, 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. The necessary data are hardwired in the code.

IFDIEL – a global switch for treating the dielectronic recombination.

• = 0 – dielectronic recombination is neglected (for bound-free transitions with smooth cross actions), or is included automatically (for transitions with cross sections that include resonances);

• ≠ 0 – dielectronic recombination is considered using the procedure and data mentioned above.

DEFAULT: IFDIEL=0

12.4 Occupation probabilities and pseudocontinua

Calculation of the occupation probabilities and related pseudocontinuum opacities is controlled by the positional parameter IFWOP imported in the atomic data file – see § 11.1 (switching on occupation probabilities), and positional parameters MODE and FR0PC – see § 11.2 (pseudocontiua). The following keyword parameters only provide additional options that can be used mostly for testing.

BERGFC – a switch for using the so-called Bergeron empirical factor (see Paper II, § 2.6)

• = 2 – this value represents the Bergeron suggestion, which is now obsolete in the context of current TLUSTY.

DEFAULT: BERGFC=1

CUTLYM – a switch for resetting the frequency cutoff for the Lyman pseudocontinum

• = 0 - no resetting, the cutoff remains as specified by the hydrogen atomic data file;

• > 0 - the cutoff is reset to the value of CUTLYM [in s^{-1}].

DEFAULT: CUTLYM=0.

CUTBAL – a switch for resetting the frequency cutoff for the Balmer pseudocontinum

• = 0 - no resetting, the cutoff remains as specified by the hydrogen atomic data file;

• > 0 - the cutoff is reset to the value of CUTBAL [in s^{-1}].

DEFAULT: CUTBAL=0.

12.5 Compton scattering

We employ a numerical procedure outlined by Hubeny et al. (2001), and described in detail in Paper II, Appendix A6 (formal solution) and C3 (linearization). First, we describe keyword parameters that define a general setup:

ICOMPT – the basic switch for including Compton scattering.

• = 0 – Compton scattering is not included; electron scattering is treated as coherent, Thomson, scattering;

• > 0 – Compton scattering is included. In this case, several other keyword parameters take effect – see below.

DEFAULT: ICOMPT=0

ICOMRT – a flag for setting the method of solution of the explicit angle-dependent transfer equation with Compton scattering

• = 0 – formal solution done by the Feautrier method.

• ≠ 0 – formal solution done by the Discontinuous Finite Element (DFE) method.

DEFAULT: ICOMRT=0

ICHCOO – a switch for selecting the treatment of frequency derivatives and boundary conditions in frequency:

• = 0 – frequency derivatives and boundary conditions in frequency are treated as described in Hubeny et al. (2011)

• > 0 – frequency derivatives and boundary conditions in frequency are treated as described in Chang & Cooper (1970)

DEFAULT: ICHCOO=0

FRLCOM – takes effect only if ICOMPT > 0 (Compton scattering is included), and then it sets the critical frequency above which all the frequency points are set to the linearization mode, regardless of the original setting specified by keyword parameter IJALI.
DEFAULT: FRLCOM=8.2E14

KNISH – if set to a non-zero value, switches on the Klein-Nishina form of the scattering cross section, however still within the framework of the Kompaneets approximation. The cross section has the form (e.g., Rybicki & Lightman 1979)

$$\frac{4}{3}\frac{\sigma(x)}{\sigma_{\rm e}} = \frac{1+x}{x^3}\left[\frac{2x(1+x)}{1+2x} - \ln(1+2x)\right] + \frac{\ln(1+2x)}{2x} - \frac{1+3x}{(1+2x)^2}, \quad (4)$$

where $\sigma_{\rm e}$ is the Thomson cross section. This approach is not fully consistent, and is used for testing purposes only.
DEFAULT: KNISH=0

The following parameters switch on various, mostly unphysical, approximations, that may sometimes be used to avoid numerical problems, or for various testing purposes.

ICOMST – a switch to specify the treatment of stimulated emission part of the source function with Compton scattering.
- $= 0$ – the stimulated emission term in the Compton scattering source function is neglected. This is useful only for testing and comparison purposes.
- > 0 – stimulated emission is included; moreover the numerical value sets the number of internal iterations of solving the fully coupled implicit transfer equation (see Paper II, Appendix A6).

DEFAULT: ICOMST=1

ICOMDE – if set to 0, the frequency derivative terms in the Compton source function are neglected. This is an unphysical option, but sometimes useful for testing purposes.
DEFAULT: ICOMDE=1

ICOMVE – a switch for inhibiting an update of the Eddington factors as a result of a solution of the angle-dependent transfer equation with Compton scattering.
- $= 0$ – Eddington factor is not updated, and is kept to the value determined from the previous solution.
- > 0 – Eddington factor is updated.

DEFAULT: ICOMVE=0

ICMDRA – a switch for linearizing the Compton scattering terms in the radiative equilibrium equation with respect to the mean intensities.
- $= 0$ – the tern is not linearized (which is sometimes more stable)
- $\neq 0$ – the term is linearized.

DEFAULT: ICMDRA=0

As explained in Paper II, Appendix A6, the overall formal solution can be done in several different ways. To provide a flexible scheme, we have introduced five keyword parameters, NCFOR1, NCFOR2, NCFULL, NCITOT, and NCCOUP, described below, to set up the procedure of the formal solution.

The following parameters control the subroutine `RTECOM` which is the basic routine for performing the formal solution of the transfer equation for all frequencies at the current values of the state parameters. The procedure is composed of several steps:

(i) An (optional) preparatory loop consisting of several (NCFOR1) iterations of solving the angle-dependent explicit transfer equation, Eq. (320) or (321) of Paper II, depending on whether the Feautrier of the DFE scheme is used (which is determined by parameter ICOMRT). This is done by subroutine `RTECF1`.

(ii) A general iteration loop that is composed of NCFULL iterations. This loop consists of two parts:

- a solution of the fully coupled (in frequency and depth) implicit transfer equation; possibly with ICOMST internal iterations to update the stimulated emission term (subroutine `rtecmc`),
- a nested iteration loop, with NCITOT iterations, which again is composed of
  - another (optional) nested iteration loop of NCCOUP iterations, each performing an explicit solution of the transfer equation [Eq. (318) of Paper II] to update the mean intensities of radiation with a fixed Eddington factor,
  - a loop of NCFOR2 iterations of explicit angle-dependent solutions of the transfer equation, Eq. (320) or (321) of Paper II.

NCFOR1 – see above
DEFAULT: NCFOR1=0

NCFOR2 – see above
DEFAULT: NCFOR2=1

NCCOUP – see above
DEFAULT: NCCOUP=0

NCITOT – see above
DEFAULT: NCITOT=1

NCFULL – see above
DEFAULT: NCFULL=1

12.6 Additional convection parameters

Here we describe several less important, or rarely used keyword parameters for treating convection.

ILGDER – a switch for the numerical representation of the mid-grid point values and for evaluating the logarithmic gradient ∇:

• $= 0$ – the mid-point values between depth points d and $d-1$ (for instance of the temperature), and the logarithmic gradient are computed ass

$$T_{d-1/2} = (T_d + T_{d-1})/2, \quad \text{and} \quad \nabla_d \equiv \nabla_{d-1/2} = \frac{T_d - T_{d-1}}{P_d - P_{d-1}} \frac{P_d + P_{d-1}}{T_d + T_{d-1}}. \tag{5}$$

• $\neq 0$

$$T_{d-1/2} = \sqrt{T_d T_{d-1}}, \quad \text{and} \quad \nabla_d = \ln(T_d/T_{d-1})/\ln(P_d/P_{d-1}) \tag{6}$$

DEFAULT: ILGDER=0

IPRESS – a flag for treating the total pressure in the convection zone:

• $= 0$ – total pressure is held fixed when evaluating the derivatives of the convective flux;

• $= 1$ – the derivatives w.r.t. the total pressure are calculated.

DEFAULT: IPRESS=0

IPRINT – a flag that controls a diagnostic output for models with convection:

• $= 0$ – no additional output, only the final model is printed;

• $= 1$ – the convective flux and the results of routine CONCOR are printed after each iteration.

DEFAULT: IPRINT=0

ITMCOR – if set to a non-zero value, it switches on an old procedure (now essentially obsolete) that correct the temperature in the convection zone if the convective flux, corresponding to the newly determined temperature and the logarithmic gradient ∇, is larger than the total flux. If so, the temperature is modified by an iterative procedure for determining new temperature that yields the convective flux that does not exceed $\sigma T_{\rm eff}^4$.

DEFAULT: ITMCOR=0

IDCONZ – a parameter for artificially switching off convection for upper layers, where the radiation pressure contribution may lead to spurious convection. IDCONZ indicates the depth index above which (i.e., for depth index $d \leq$ IDCONZ), the convection is switched off regardless of the values of the actual and the adiabatic gradient.

DEFAULT: IDCONZ=31

DERT – the value of $\Delta T/T$ for a numerical evaluation of derivatives of the convective flux with respect to temperature. It takes effect only in the Rybicki scheme (if IFRYB > 0). (Notice that when a standard scheme is used, the value of $\Delta T/T$ is hardwired at 0.001.)

DEFAULT: DERT=0.01

12.7 State equation and thermodynamic quantities

Here is a summary of keyword parameters, useful mostly for testing purposes:

IIRWIN – a mode of using the Irwin partition functions tables. In any case, they are used only for $T \leq 16000$ K.
- $= 0$ – Irwin tables are only used when molecules are taken into account in the equation of state (IFMOL > 0);
- > 0 – Irwin tables are used by default (even for IFMOL=0);

DEFAULT: IIRWIN=0

IFTENE – a mode of evaluating the internal energy – see Paper II, Appendix B3;
- ≤ 1 – the internal energy only contains the ionization energies;
- > 1 – the internal energy also contains contributions from the partition functions, $d \ln U / d \ln T$.

DEFAULT: IFTENE=0

IFENTR – a mode of evaluation of the the specific heat and the adiabatic gradient
- $= 0$ – standard evaluation through the T, P, and internal energy;
- > 0 – an evaluation through the T, P, and entropy.

DEFAULT: IFENTR=0

12.8 Details of accretion disks

As shown in Paper II, § 2.2.2, the (generally depth-dependent) kinematic viscosity w is allowed to vary as a step-wise power law of the column mass density, viz.

$$w(m) = w_0 \, (m/m_0)^{\zeta_0} \, , \quad m > m_{\rm d} \, , \tag{7}$$

$$w(m) = w_1 \, (m/m_0)^{\zeta_1} \, , \quad m < m_{\rm d} \, , \tag{8}$$

where m_0 is the column mass at the mid-plane, and $m_{\rm d}$ is the column mass at the so-called division point, which is an input parameter. With this parametrization, 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

There are thus four independent parameters: the power law exponents ζ_0 and ζ_1, the division point, $m_{\rm d}$; and f, the fraction of energy dissipated in deep layers where $m > m_{\rm d}$. 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 $\int_{m_{\rm d}}^{m_0} w(m) dm/m_0 = f \, \overline{w}$. We obtain

$$w_0 = \frac{f \, \overline{w} (\zeta_0 + 1)}{1 - (m_{\rm d}/m_0)^{\zeta_0 + 1}} \, , \tag{9}$$

$$w_1 = \frac{(1 - f) \, \overline{w} (\zeta_1 + 1)}{(m_{\rm d}/m_0)^{\zeta_1 + 1}} \, . \tag{10}$$

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

$$\frac{m_{\rm d}}{m_0} = \left(1 + \frac{\zeta_0 + 1}{\zeta_1 + 1} \frac{f}{1-f}\right)^{-\frac{1}{\zeta_0+1}} . \tag{11}$$

Typically, the deep-layer power law exponent ζ_0 is set to 0 (constant viscosity), while the "surface" power law exponent ζ_1 is sometimes 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;.

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

ZETA1 – the viscosity parameter ζ_1
DEFAULT: ZETA1=0 (viscosity is 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);
- > 0 – the value of f (must obviously be between 0 and 1)
- < 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 $m_0/m_{\rm tot}$, where $m_{\rm tot}$ 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 – a 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 mid-plane is computed in the LTE-grey model (or read from the input model), and subsequently held fixed.
- $= 1$ – the basic scale is the z-scale. It is not a recommended option.

DEFAULT: IZSCAL=0

IFZ0 – this keyword has two functions: (i) it is a switch for treating the lower boundary condition for the radiative transfer equation for disks; and (ii) it indicates a number of global iterations for which the z-scale is being recalculated in the formal solution. This number is determined by the absolute value of IFZ0.
- ≥ 0 – lower boundary condition is a symmetry boundary condition given by Eq. (52) of Paper II;

• < 0 – lower boundary condition is represented by the diffusion approximation, Eq. (5) of Paper II.
DEFAULT: IFZ0=9 (but reset to -1 for atmospheres)

IBCHE – a mode of treating the upper boundary condition of the vertical hydrostatic equilibrium equation:
• $= 0$ – the boundary condition is the same as in the case of stellar atmospheres;
• $= 1$ – the boundary condition is in the form derived specifically for disks, expressed as – see Paper II, § 4.2,

$$m_1 = H_g \rho(z_1) f[(z - H_r)/H_g], \tag{12}$$

where $f(x) = (\sqrt{\pi}/2) \exp(x^2) \operatorname{erfc}(x)$, and H_g and H_r are the gas pressure scale height and radiation pressure scale height, respectively.
• $= 2$ – the same expression as above, but a different (older) variant of its linearization, namely with the scale heights H_g and H_r held fixed. This is an outdated option.
DEFAULT: IBCHE=1

ICOMGR – a switch for a treatment of Compton scattering in the LTE-gray starting model
• $= 0$ – the Compton scattering is neglected in the LTE-gray model;
• $= 1$ – the Compton scattering is taken into account in evaluating the LTE-gray model, using the procedure described in Paper II, § 4.2, Eqs. (185) – (186).
DEFAULT: ICOMGR=0

12.9 Additional, approximately described physical processes

Here we describe several processes that are not a main emphasis of TLUSTY, but can be included in an approximate way.

12.9.1 Approximate partial frequency redistribution

There are two keywords that control the adopted treatment of partial redistribution:

IFPRD – switch for treating the four lines with approximate partial redistribution;
• $= 0$ – no partial redistribution, all lines are treated with complete redistribution;
• > 0 – partial redistribution in all four lines considered by TLUSTY (Lα, Mg I and Mg II resonance lines) is switched on.
DEFAULT: IFPRD=0

XPDIV – division frequency (in units of Doppler width) for the partial coherent scattering approximation.
DEFAULT: XPDIV=3.

12.9.2 Wind blanketing

This approximation, introduced by Abbott and Hummer (1985), and slightly modified by Voels et al. (1988), mimics an influence of atmospheric layers outside the uppermost depth point, presumably a stellar wind, by a frequency-dependent albedo that specifies the portion of radiation reflected back due to the wind. It attains values between 0 and 1.

This approach is relatively obsolete and is kept mostly for historical reasons. Here are the parameters that sets the treatment of the wind albedo:

IWINBL – a switch indicating whether the wind-blanketing albedo is considered.
- $= 0$ – 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

DEFAULT: IWINBL=-1

ALBAVE – frequency-integrated wind blanketing albedo for constructing a starting LTE-gray model.
DEFAULT: ALBAVE=0 (no wind blanketing)

13 Keywords for additional numerical options

In this chapter we describe a number of keyword parameters that control various aspects of the numerical setup of model atmosphere calculations.

13.1 Working with opacity tables

As stated in § 7.4.1, using the opacity table is switched on by the keyword IOPTAB. The table has the following structure:
- 1st record: number of frequencies (NUMFREQ), temperatures (NUMTEMP), and densities (NUMRHO)
- 2nd record: vector of logarithms of temperatures (TEMPVEC)
- 3rd record: vector of logarithms of densities (RHOVEC)
- NUMFREQ blocks containing: the frequency, and subsequently NUMRHO sub-blocks of NUMTEMP values of log(opacity).

The maximum number of temperatures and densities is given by parameters MTABT and MTABR, set in the INCLUDE file `BASICS.FOR` to 50. This is also the number of actual temperatures and densities in the current table

`absopac.dat`. The maximum number of frequencies, MFRTAB, is also specified in `BASICS.FOR`. In the standard setup, where the opacity table is not used, MFRTAB is set to 1 to save memory, so when the opacity table is being used, this number should be so to at least the current number of frequencies in the table, such as MFRTAB=30000 (which is the statement commented out in the distributed file `BASICS.FOR`; the actual distributed `absopac.dat` has NUMFREQ=28706.

The opacity table is distributed as an ASCII file, but there is a simple program (`optabtr.f`) that transfers it to the binary format. Reading the binary opacity table is much faster, so when computing many models it is advantageous to use the binary format. The format is controlled by the keyword IBINOP.

The opacity table is read at the beginning of calculations. The first step is to interpolate the opacity from the internal frequencies of the table to the frequency points actually used, for each pair of temperature and density given by TEMPVEC and RHOVEC. This avoids the necessity of repeated interpolations in frequency during the calculations, so one interpolates only in temperature and density.

There are several additional options:

IBINOP – a switch for the format of the opacity table.
- $= 0$ – opacity table is in the ASCII format;
- $= 1$ – opacity table is in the binary format.

DEFAULT: IBINOP=1

IFRSET – a switch for resetting the frequency points used in the linearization (which are otherwise given by the positional parameter NFREAD and several keyword parameters such as FRCMAX, described in § 7.4.2) when using the opacity table.
- $= 0$ – frequency points are not reset, and are given as specified independently of the opacity table;
- > 0 – the frequency points used in the linearization are reset to the tabular frequencies. No interpolation in frequency is thus needed.

DEFAULT: IFRSET=0

13.2 Details of the formal solution

The *formal solution*, as discussed in physical terms in Paper II, § 3.8, and Appendix B, is a set of calculations between two consecutive iterations of the global linearization scheme. It can influence the performance of the code significantly. In the code, it is driven by subroutine `RESOLV`, which calls a number of additional subroutines. The formal solution has several basic steps:

(i) Computing new components of the state vector after completing of a previous global linearization iteration (subroutine `INITIA`);

(ii) update of temperature (in particular when convection is taken into account);

(iii) update of density and pressure (and the vertical distance from the mid-plane in case of disks);

(iv) update of level populations and radiation field.

Steps (ii) - (iv) may be iterated several times, and steps (ii) - (iii) may be missing altogether for certain models.

Below, we describe these steps and the corresponding keyword parameters that control a detailed setup of the global formal solution.

(i) Computing new components of the state vector

By default, this is done, as explained in Paper II, § 3.1,

$$\psi_{di}^{(n)} = \psi_{di}^{(n-1)} + \delta\psi_{di}^{(n)}, \tag{13}$$

where the superscript denotes the iteration number. This can be done for all components of the vector ψ; however, it was found already in the early days of computing NLTE model atmospheres that in some cases it is better to use a different approach. This is controlled by the following keyword parameters:

IFPOPR – a switch for treating the calculation of new populations just after completing an iteration of the linearization scheme.

- $= 0$ – the original Auer-Mihalas scheme: after a completed linearization iteration, new populations (i.e. those obtained as $n^{\rm new} = n^{\rm old} + \Delta n$) are not used; instead one uses a new radiation field to compute new radiative rates, and the populations are determined by solving the rate equations. The option is kept for historical reasons; it is only useful for the pure complete linearization scheme.
- > 0 – the populations 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

ITEMP – a flag for evaluating the "new" temperature when convection is taken into account:

- $= 0$ – new temperature is calculated as $T^{\rm new} = T^{\rm old} + \delta T$ (i.e., exactly as it is done without convection);
- $= 1$ – new temperature is calculated through the logarithmic gradient ∇ in the convection zone;
- $= 2$ – new temperature is calculated through ∇ everywhere.

DEFAULT: ITEMP=0

(ii) Update of temperature

It should be kept in mind that the temperature is the critical quantity of a model, on which the other state parameters depend sensitively. If the temperature is seriously wrong at some points in the atmosphere, it is likely that the whole

procedure based on a linearization scheme will diverge, or at least converge slowly. A care should therefore be taken to assure that the "new" temperature is as consistent with other state parameters, and behaves as smoothly, as possible. There are two types of correction procedures, (i) numerical smoothing, and (ii) physical corrections, based on the solution of an energy balance equation. The first category is controlled by the following flag:

IOSCOR – if set to a non-zero value, it invokes a procedure for smoothing a possible oscillatory behavior of the new temperature after a completed iteration of the linearization scheme (subroutine `OSCCOR`). The absolute value of IOSCOR specifies the index of the deepest depth point at which is the correction procedure performed. The routine finds the limiting depth indices of the region where the oscillations occur, $d_{\min}$ and $d_{\max}$, and sets the new temperature in this region by interpolating in logarithms,

$$\log T_d^{\rm new} = \log T_{d_{\min}} + \frac{\log(T_{d_{\max}}/T_{d_{\min}})}{\log(m_{d_{\max}}/m_{d_{\min}})} \log(m_d/m_{d_{\min}}), \qquad (14)$$

• if < 0, then in addition the program finds the minimum temperature, and resets the local new temperature for all depths above the minimum (lower depth indices) to the minimum temperature.
DEFAULT: IOSCOR=0

There is a number of flags controlling the update of temperature in the convection zone; they are described in detail in § 7.8 and § 12.6.

(iii) Update of density and pressure

There are several flags in this category; their action differs depending on whether one computes a model atmosphere or a vertical structure of a disk.

IHECOR – a mode of treating the total particle density N during the global formal solution:
• $= 0$ – the total particle density is held fixed;
• > 0 – the total particle density is recalculated by solving the hydrostatic equilibrium equation with the current values of the other state parameters (T, radiation intensities).
DEFAULT: IHECOR=0

IHESO6 – if set to a non-zero value, it activates a special procedure (subroutine `HESOL6`) in the formal solution for a simultaneous solution for six variables – P, $P_{\rm gas}$, ρ, N, $n_{\rm e}$, and z by solving the hydrostatic equilibrium equation, the definitions of P, $P_{\rm gas}$, and ρ, and the z-m relation – see Paper II, Appendix B4. It operates only for disks.
DEFAULT: IHESO6=0

(iv) Update of level populations and radiation field

As discussed in Paper II, § 3.8, this is the most important step of the global formal solution that lies at the very heart of the NLTE approach. This step is

sometimes called the "restricted NLTE problem", which represents a simultaneous solution of the kinetic equilibrium and the radiative transfer equations to determine the level populations and the radiation intensities, with other state parameters held fixed. In the original approach one used a simple Lambda iteration procedure, while in the present version one uses a more efficient procedure based on the ALI scheme with preconditioning – see Paper II, Appendix B1.

We summarize here the corresponding keyword parameters that control this procedure. Parameter NLAMBD was already described in § 7.4.6.

NLAMBD – number of iterations for solving the coupled radiative transfer and kinetic equilibrium equation of the global formal solution. Historically, these were ordinary Lambda iterations, hence the name NLAMBD. The current default procedure is instead the ALI scheme with preconditioning.
DEFAULT: NLAMBD=2 for NLTE models; NLAMBD=1 for LTE models

CHMAXT – a parameter that enables to change the number of iterations of the global formal solution (given by NLAMBD) when the model is almost converged. If the maximum of the absolute values of the relative changes of temperature at all depths decreases below CHMAXT, the number of iterations is set to NLAMT.
DEFAULT: CHMAXT=0.01

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

IFPREC – a flag for treating the preconditioning of the statistical equilibrium equations (after Rybicki & Hummer 1991):
• $= 0$ – no preconditioning;
• $= 1$ – a diagonal (local) preconditioning, as described in Paper II, Appendix B1, is switched on;
• > 1 – a tri-diagonal (non-local) preconditioning is switched on (this option is not supported in version 205, and thus should not be used).
DEFAULT: IFPREC=1

IACPP – a switch for invoking the 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), then no acceleration is performed.
DEFAULT: IACPP=7

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

IELCOR – a flag for turning off an iterative update of the electron density by solving iteratively a non-linear system of the kinetic equilibrium equations

and the charge conservation equation. IELCOR has the meaning of the serial number of the global iteration till which is this procedure performed.
DEFAULT: IELCOR=100 (i.e. ELCOR is called always)

13.3 Additional parameters for LTE-gray models

These are mostly obsolete parameters, kept for downward compatibility, and for possible comparisons with other modeling approaches and codes.

TSURF – a mode of evaluating the surface temperature:
- $= 0$ – the surface temperature (T_0) and the Hopf function (q_0) are evaluated exactly, that is, $T_0 = [(3/4)q_0)]^{1/4} T_{\rm eff}$, with $q_0 = 1/\sqrt{3}$, so $T_0 = 0.8112\, T_{\rm eff}$;
- > 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 the LTE-grey model.
- if = 0 – NDGREY is set to ND

DEFAULT: NDGREY=0

IDGREY – a mode of determining the mass-depth scale to be used in the subsequent linearization:
- $= 0$ – the depth grid m_d (in g cm^{-2}) is evaluated as a column mass corresponding to the 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.
- $= 1$ – similar, but now m_d 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, read at the end of the standard input (unit 5) file.]. This option is similar to IDGREY=0, but now TAU1 and TAUL may be different from TAUFIR and TAULAS. This option is now obsolete.

DEFAULT: IDGREY=0

IHM – if non-zero, the negative hydrogen ion is considered in the particle and charge conservation when constructing an LTE-gray model;
DEFAULT: IHM=0

IH2 – if non-zero, the hydrogen molecule is considered in the particle and charge conservation when constructing an LTE-gray model;
DEFAULT: IH2=0

IH2P – if non-zero, the ionized hydrogen molecule is considered in the particle and charge conservation when constructing an LTE-gray model
DEFAULT: IH2P=0

13.4 Setup of the radiative transfer equation and Λ^* operator

Here we describe some additional parameters for the setup of the transfer equation and the evaluation of the approximate Λ^* operator. These are rarely used, and if so then mostly for testing and comparison purposes. Their default values usually yield the best results.

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

DJMAX – the maximum relative change of the mean intensity in the internal ALI iteration loop for treating electron scattering in the case of the DFE formal solution. It has an effect only if ISPLIN=5.
DEFAULT: DJMAX=0.001

NTRALI – the maximum number of iterations of the internal ALI iteration loop for treating electron scattering in the case of the DFE formal solution. It has an effect only if ISPLIN=5.
DEFAULT: NTRALI=3

ILMCOR – a mode of including the electron scattering contribution to the approximate Lambda operator Λ^*:
• = 0 – the Λ operator is defined to act 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 is the scattering coefficient, $\sigma = n_{\rm e}\sigma_{\rm e}$, with $\sigma_{\rm e}$ being the electron scattering cross section.
• = 1 – the Λ operator is defined to act on the thermal source function $\mathcal{S}^{\rm th} = \eta/\kappa$, i.e. $J = \Lambda[\eta/\kappa]$.
DEFAULT: ILMCOR=1

ILPSCT – a mode of including the electron scattering correction in the preconditioning scheme:

• = 0 – the Λ operator is defined to act on the thermal source function;
• = 1 – the Λ operator is defined to act 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 Λ operator is defined to act on the thermal source function;
• = 1 – the Λ operator is defined to act on the source function of the form $S = \eta/(\kappa + \sigma)$.
DEFAULT: ILASCT=0

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

13.5 Setup of the kinetic equilibrium equations

Similarly to § 13.4, we list here several less used keyword parameters that control the setup of the kinetic equilibrium equation; the more important parameters were already described in § 7.4.4.

MODREF – a flag for setting up the reference levels of the individual explicit species. Recall that the reference level is the energy level for each species for which the kinetic equilibrium equation is replaced by the abundance definition equation. The indices of the 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 positional parameter IMODL (§ 11.1), and is not changed;
• > 0 – the mode is reset, for all levels except the highest ionization stage, to IMODL=1, i.e. the updated LTE mode.
DEFAULT: IFLEV=0 for NLTE; IFLEV=1 for LTE models

ICHC – switch for selecting the closing equation for the set of kinetic equilibrium equations:
- = 0 – the closing equation is the abundance definition 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 the kinetic equilibrium equations:
- = 0 – kinetic equilibrium equations for all species are solved simultaneously (with one big rate matrix);
- = 1 – kinetic 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

POPZR2 – a secondary parameter for setting up a level zeroing.
DEFAULT: POPZR2=1.e-20

13.6 Auxiliary, mostly obsolete, parameters

IFMOFF – a flag for considering the modified free-free cross section for all explicit ions even if the atomic data files do not specify it. If set to a non-zero value, the characteristic quantum number is set to the main quantum number of the highest level of an ion + 1.
DEFAULT: IFMOFF=0

IOVER – a flag for turning on the "line-overlapping" mode:
- = 0 – no overlapping is allowed for (only one line may contribute to the 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

IBFINT – a mode of storing the photoionization cross sections:
- = 0 – means that the cross sections are stored for all frequency points;
- = 1 – means that the 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 kinetic equilibrium equations in the hybrid CL/ALI scheme:
- $= 0$ – the rate equations in the CL/ALI scheme are not linearized;
- > 0 – the rate equations in the CL/ALI scheme are linearized; there are several variants of treating 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 the 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 the 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 set to zero.
- > 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 $\delta(\psi_i)/\psi_i = \max[1/\mathrm{DPSILG} - 1, \delta(\psi_i)/\psi_i]$, and $\delta(\psi_i)/\psi_i = \min[\mathrm{DPSILG} - 1, \delta(\psi_i)/\psi_i]$;
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 DPSILG.
DEFAULT: DPSILT=1.25

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

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

13.7 Collisional-radiative switching

This is an obsolete procedure suggested originally by Hummer & Voels (1988), somewhat modified by considering a depth-dependent switching parameter. It consists in artificially multiplying the radiative rates by a factor CRSW, which satisfies CRSW < 1, and gradually increase this factor until it reaches unity. This procedure may lead to a greater stability of the kinetic equilibrium equations. The actual setup is controlled by the following keywords:

ICRSW – switch for turning on the collisional-radiative switching;
- $= 0$ – collisional-radiative switching is not considered;
- > 0 – collisional-radiative switching is considered.

DEFAULT: ICRSW=0

SWPFAC sets the initial CRSW=SWPFAC $\times$ min(collis.rate/rad.rate)
DEFAULT: SWPFAC=0.1

SWPLIM – a limiting factor for CRSW; in the sense that
if CRSW $>$ SWPLIM, then CRSW $= 1$,
DEFAULT: SWPLIM=0.001

SWPINC – an increment factor for determining new CRSW, namely
CRSW(actual) = CRSW(previous) $\times$ SWPINC
DEFAULT: SWPINC=3.

13.8 Parameters determining the 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 § 9.2
DEFAULT: IPRIND=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 § 9.2.
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 useful quantities for all continuum frequencies is generated.
- $= 1$ – stores the opacity for all continuum frequencies as a function of depth (Unit 85)
- $= 2$ – stores the absorption, scattering, emission coefficients, and the mean intensity for all continuum frequencies, as a function of depth – see § 9.2.

DEFAULT: IPOPAC=0

ICOOLP – if set to a non-zero value, the net total cooling rate is stored as a function of depth (Unit 87); if moreover it is set to a vale > 10, also the individual cooling rates for all explicit ions are also stored (Unit 88) – see § 9.2.
DEFAULT: ICOOLP=0

14 User-supplied routines

To help the user to implement his/her own expressions for various atomic parameters, we have set up a number of dummy routines that are prepared to accept the user supplied expressions. In this way the user does not have to worry about where exactly to place the desired expression, and about possible indirect effects of the new piece of code. Also, the user does not have to understand the detailed structure of the code.

There are four such routines which are described below.

14.1 `SPSIGK` – non-standard photoionization cross sections

The routine is called with the following parameters:

```
SUBROUTINE SPSIGK(IB,FR,SIGSP)
```

The input parameters are:

- `IB` is the switch given by the input parameter IFANCY (renamed to IBF), which has to be negative to activate this routine – see § 11.2,. The actual value of IB invokes one particular expression or a hardwired table. We have already used the following values to invoke some special formulae or tables:
  - IB = −602 – an outdated formula for the He I ground state;
  - IB = −202 – another outdated formula for the He I ground state;
  - IB = −602 – special table of cross section for C I $2p^2\ ^1D$ level (provided by G.B. Taylor, priv. communication);
  - IB = −603 – special table of cross section for C I $2p^2\ ^1S$ level (G.B. Taylor, priv. communication);
  - between −101 and −137 – cross section after Hidalgo (1968). In this case, −IB−100 is the Hidalgo's index;
  - between −301 and −337 – cross section after Reilman & Manson (1979). Again, −IB−300 is their index.

  Any other values are free and available for the user.
- `FR` is the frequency [in s^{-1}],

The output is `SIGSP` [in cm $^{-2}$].

14.2 `GAMSP` – non-standard Voigt damping parameters

The routine is called with the following parameters:

```
SUBROUTINE GAMSP(ITR,T,ANE,AGAM)
```

The subroutine is called if the input parameter GAMAR (see § 11.3) is coded negative. The input parameters are:

- `ITR` is the index of the transition,
- T is the temperature [K],
- `ANE` is the electron density [cm $^{-3}$].

The output is `AGAM` the Voigt parameter, a, where $a \equiv \Gamma/(4\pi\Delta\nu_D)$, where Γ is the (physical) damping parameter, and $\Delta\nu_D$ is the Doppler width.

14.3 `CSPEC` – non-standard collisional rates

The routine is called with the following parameters:

```
SUBROUTINE CSPEC(I,J,IC,OS,CP,U0,T,CS)
```

The input parameters are:

- `I,J` – indices of the lower and the upper level of the transition;
- `IC` – a collisional switch, given by the input parameter ICOL, which must be set negative to invoke this routine – see § 11.3. The following values are already used:
  - IC= -1, already mentioned in § 11.3, is reserved for the van Regemorter formula for neutral atoms;
  - IC= -2 – a usual van Regemorter formula for ions. This is a redundant option because this formula is invoked by setting ICOL=0 without a need to call this special routine.
- `OS` – oscillator strength; given by the input parameter OSC0;
- `CP` – collisional parameter, given by the input parameter CPARAM – see § 11.3;
- `U0` – the value of $U_0 = h\nu_0/kT$;
- `T` – temperature [K].

The output is `CS`, the collisional rate Ω – see § 11.3.

14.4 `PFSPEC` – non-standard partition functions

The routine is called with the following parameters:

```
SUBROUTINE PFSPEC(IAT,IZI,T,ANE,U,DUT,DUN)
```

The subroutine is called if the input parameter MODPF (see § 4.2) is set to a negative value. The input parameters are:

- `IAT` – atomic number;
- `IZI` – ionization stage (IZI=1 for neutrals, etc.);
- `T` – temperature [K];
- `ANE` – electron density [cm $^{-3}$].

The output is `U`, the partition function, and its derivatives with respect to temperature and electron density, respectively (`DUT` and `DUN`); the derivatives are usually set to 0.

15 Summary of useful tricks; troubleshooting

TLUSTY can employ 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. These approaches prove useful in some cases, but in some other cases they may harm the convergence or even lead to additional numerical problems. Consequently, they should not be used blindly.

The keyword parameters that switch on/off such options are set to their default values and may be changed by setting an appropriate value in the keyword parameter 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 have to 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 describe 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 Chap. 11

This chapter will present an explanation of many optional keyword parameters introduced above. The previous chapters 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 invoking purely numerical tricks; (ii) parameters that influence the accuracy of a 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 below.

15.1 Purely numerical tricks

These procedures are defined as that their use does not change the accuracy of 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).

- *Setup 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 line, and the central frequency in Lβ and Lγ lines, together with the first three points in the He II Lyman continuum are set to linearized mode; the rest of the frequencies are in the ALI mode.
  There is also a useful keyword IFRALI (see § 7.4.3) which can change the setup globally.

- *Rybicki scheme*
  Setting this scheme is in a large majority cases preferable for LTE models. Surprisingly, it can also be used cautiously for NLTE models in case of convergence problems. As discussed in Paper II, § 3.3, the scheme is not designed for computing full NLTE models, but can serve as a means to compute intermediate NLTE model from which the final model may be converged more easily. An actual example of using the Rybicki scheme in the context of NLTE models was shown in § 6.5.

- *Accelerations*
  There are two basic acceleration schemes: Ng and Kantorovich, see Paper II, § 3.4. The corresponding keywords are described in § 7.4.8. Both accelerations are helpful tools to speed up calculations considerably, or even sometimes to improve convergence properties, but on the other hand they may cause problems in some cases. Therefore, they should be used with caution.

  As demonstrated in § 10.2, 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 and the acceleration is done too soon, the consequence is often a harmful or disastrous effect upon the convergence. If it is done too late it does not do what it could, namely speed up the calculations. In some cases the Ng acceleration is crucial even for the success of the run; it is when the normal linearization produces undamped oscillations, so that only the 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 the 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.

An analogous warning can be expressed about the Kantorovich scheme, whose onset is controlled by the keyword parameter ITEK. Turning it on too soon may slow down the convergence; or lead to divergence, turning it on too late would not do any harm to the convergence rate, but increases the execution time significantly. Again, it is very dangerous to use it for convective models, unless starting it late in the iteration process when the position of the convection zone does not change any more, but in such a case it does not lead to a significant reduction of the computer time. Therefore, a safe strategy is to turn it off completely for convective models.

- *Level grouping*
  This numerical trick may significantly reduce the number of level populations to be linearized – see Paper II, § 3.7. We remind that a level group is a set of several 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 the linearization. In the formal solution step, one solves for all the individual level populations exactly. The grouping is set up by the atomic data files (parameter IMODL; see Sect. 11.1). 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 the radiative transfer formal solver*
  This is driven by keyword ISPLIN (see § 7.4.3). Usually, the original 2nd-order Feautrier scheme (ISPLIN=0; the default) works very well. One exception is the case of a strong external irradiation; in this case setting ISPLIN=5 (the DFE scheme) may be preferable.

- *Number of iterations of the global formal solution ("Lambda" iterations)*
  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. An actual example is shown in § 10.2.4.

- *Choice of the approximate Λ^*-operator*
  This is driven by keywords IFALI (see § 7.4.3) – 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 supported, and may not work properly in some cases.

- *Choice of the so-called "reference atom" and the reference levels*
  This is driven by keyword IATREF and MODREF (see § 7.4.4 and § 13.5). 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).

- *Limiting the values of the relative changes to be used to the obtain next iterates of the structural parameters*
  This is driven by keywords DPSILT, DPSILG, DPSILN, DPSILD – see Sect. 13.6. Usually, the default values work well.

15.2 Changing the accuracy of a model

There are parameters In this category that are originally meant to influence the accuracy of a 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 recommended to decrease the value to ND=50, which saves computer time and memory without a decrease of the accuracy of the model. In fact, this was used in our recent O-star and B-star model grid calculations – Lanz & Hubeny (2003, 2007).

- *Setting up the minimum and maximum Rosseland optical depth for a model* (only if the model is computed from scratch)
  This is driven by the keywords TAUFIR and TAULAS (see § 7.5). 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 more) because hydrogen provides very little opacity in the X-ray region and thus the atmosphere is very transparent there. Another example are strongly irradiated companions of hot stars, where the external irradiation may penetrate deep into the atmospheres of the companions. Again, one may need to set TAULAS to a larger value.

- *Convergence criterion*
  It is driven by the keywords NITER and CHMAX (see § 7.4.6). We recall

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

- *Treatment of the iron-peak lines*
  This is controlled by keywords ISPODF, DDNU, STRLX, CNU1, CNU2, CHMAXT, and JIDS - see § 7.7. These parameters influence typically the accuracy of a model (and, obviously, the computer time needed to generate a model), but usually not its convergence properties.

15.3 Introducing some helpful minor physical approximations

Here, we consider 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., setting detailed radiative balance for too many lines) they would provide a model of 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:

- *Division point between the differential and integral form of the radiative equilibrium equation*
  This is driven by the keywords TAUDIV, IDLST, and NDRE – see § 7.4.5. 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). In the past, changing this value is often *the* decisive trick to make LTE models converge.

  It should be stressed that when the Rybicki scheme is used, it usually eliminates most of the problems with the radiative (or radiative/convective) equilibrium equation, and the value of TAUDIV is not so critical; in fact, it can be set to a small value (say 0.01). Also, in this case it is mandatory to set IDLST=0.

  If the Rybicki scheme is not used, there is no a priori recipe to choose the best value of TAUDIV. 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 ($T_{\rm eff} < 10,000$ K) setting TAUDIV=5 usually helps. In contrast, for accretions disks the value TAUDIV=0.05 is sometimes more advantageous. However, the user should be aware of the fact that this trick may lead to numerical inaccuracies. When a linear combination of the differential and the integral forms of the radiative

equilibrium equation is satisfied, it does not necessarily mean that both are satisfied individually. Specifically, if Eq. (16) of Paper II is satisfied exactly,

$$\alpha\left[\int_0^\infty \left(\chi_\nu J_\nu - \eta_\nu^{\rm tot}\right) d\nu\right] + \beta\left[\int_0^\infty \frac{d(f_\nu J_\nu)}{d\tau_\nu}\, d\nu - \frac{\sigma_R}{4\pi}\, T_{\rm eff}^4\right] = 0, \qquad (15)$$

one can still have

$$\alpha\left[\int_0^\infty \left(\chi_\nu J_\nu - \eta_\nu^{\rm tot}\right) d\nu\right] = -\epsilon, \qquad (16)$$

and

$$\beta\left[\int_0^\infty \frac{d(f_\nu J_\nu)}{d\tau_\nu}\, d\nu - \frac{\sigma_R}{4\pi}\, T_{\rm eff}^4\right] = \epsilon, \qquad (17)$$

so that radiative equilibrium is in fact *not satisfied*. The higher the value is set for TAUDIV, the larger the errors could be. If the user sets a value larger than the default, it is advisable to recompute the converged model with the default value of TAUDIV. In other words, increasing TAUDIV to obtain an intermediate model may enable to converge a model that would not converge directly with the default value of TAUDIV. To verify that the model is properly converged, one has to inspect the last table of the standard output (Unit 6) for the conservation of the total flux.

- *Artificial lowering of the total radiative pressure at the surface*
  Radiative acceleration increases in the superficial layers ($\tau_{\rm Ross} < 10^{-5}$), and may overcome the gravitational acceleration. The model may become numerically unstable in these layers, although physically stable at larger optical depths. The option XGRAD=0 (see § 7.9) allows to auto-limit the radiative acceleration to some fraction of the gravity in the ten uppermost layers. This is the default approach. The resulting model is not exact at the surface layers (in fact, it cannot be because one does not include a wind anyway), but is very reasonably accurate at deeper layers where most of the observed spectral features form. This option is therefore extremely useful.

  Setting XGRAD=-1., or -2., allows to impose a more stringent cut-off in the 20 uppermost layers, which may critically help the 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 should be used only with extreme caution.

- *Fixed temperature at a surface layer*
  This is set up by the parameter NRETC (see § 7.9). This 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 the first 10 depth points will

be held fixed to the values given by the input model). Once one obtains a converged solution, it is recommended to re-converge 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 the parameters FRCMIN and FRCMAX – see § 7.4.2. 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 the high-frequency tail*
  This is driven by parameters NFTAIL, DFTAIL, and CFRMAX - see § 7.4.2. 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, to increase NFTAIL.

- *Setting a detailed radiative balance in lines*
  In many cases, this trick helps to provide an intermediate model if other tricks fail. This topic was discussed at length in Chap. 10.

- *Level zeroing*
  This is a useful trick that may avoid some floating-point problems. The idea is as follows (see Paper II, § 3.7): 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^{-20}), the population is set exactly to 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 the numerical stability without compromising the final solution.

  However, a level may also be super-zeroed, if it is zeroed in all depth points. In that case it is permanently removed from the set of explicit levels and thus the number of state parameters is indeed reduced. This option is very useful for instance for hot accretion disks, where one can originally set all ions of a species, for example Fe I to Fe XXVII, and let the code decide which are going to be removed based on the actual physical conditions.

- *Zeroing of the mean intensity*
  Analogously to level zeroing, one may set the mean intensity of radiation to zero if the value of the mean intensity decreases 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 some selected structural parameters fixed*
  This is driven by the keywords described in § 7.4.7. Any of these options may be useful to compute an intermediate model in the case when convergence cannot be achieved with all structural parameters being linearized. Usually, keeping just the temperature fixed (INRE=0) will provide an intermediate converged model; in some cases it is better to also keep the electron density and the total particle density fixed; in this case one may set the shortcut parameter IFIXMO=1 – see also § 10.2.4.

15.4 Optional, but potentially important physical processes

This category of tricks allows one to remove or include some 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 in an intermediate case between a completely negligible and almost negligible influence of a given mechanism its inclusion or rejection may significantly influence the convergence properties of a model.

- *Convection*
  The parameters for switching on convection are described in § 7.2 (HMIX0, MLTYPE); and the parameters for controlling numerical details are in § 7.8, and § 12.6. If the convection is weak, it may be advantageous to converge first a model without convection; however usually it is 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 the parameters IRSCT, IOPHMI, IOPH2P – see § 12.2.1 and § 12.2.2. 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 diminished 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 examples are the Rayleigh scattering opacity (IRSCT), H_2^+ opacity (IOPH2P), and the Collision-Induced Absorption (CIA) opacity (parameter IFCIA). In the two latter cases, setting IOPH2P or IFCIA 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, for accretion disks. It is switched on by setting the parameter ICOMPT to a non-zero value. The equations, procedures, and corresponding keyword parameters are described in Paper II, Appendix A6 and C3,

and here in § 12.5. Computing a model with Compton scattering is typically slower than without it, but hot models are obviously more accurate when it is included, and in some cases it can even improve the convergence properties and the stability of the numerical scheme. For very hot models, where all species are essentially fully ionized, it is even mandatory to include the Compton scattering because it becomes the dominant agent for establishing the radiative equilibrium.

- *Microturbulence and turbulent pressure*
  Their treatment is driven by the parameters VTB and IPTURB – see § 7.2. The value of VTB does not usually influence the convergence properties of the model. On the other hand, parameter IPTURB, which controls whether the assumed microturbulence will be associated with a corresponding turbulent pressure, may influence the hydrostatic equilibrium and thus the convergence properties. In case of a high turbulence (close to, or larger than, the thermal velocity), a safer and perhaps more physical option is to set IPTURB=0, in which case there is no turbulent pressure associated with the assumed turbulent velocity.

16 List of keyword parameters

Here we give the list of all keyword parameters in alphabetic order, including their default values, and the reference to the section where they are described in detail.

keyword	default value	described in
ABPLA0	0.3	7.5
ABPMIN	10^{-5}	7.5
ABROS0	0.4	7.5
ADIST	0.	7.3
ALBAVE	0	12.9.2
ALPHAV	0.1	7.2.3
BERGFC	0.	12.4
CFRMAX	2 (0 for disks)	7.4.2
CHMAX	10^{-3}	7.4.6
CHMAXT	0	13.2
CNU1	4.5	7.7
CNU2	3	7.7
CRFLIM	0.7	7.8
CUTBAL	0.	12.4
CUTLYM	0.	12.4
DDNU	0.75	7.7
DERT	0.01	12.6
DFTAIL	0.25	7.4.2
DION0	1.	13.3

DJMAX	0.001	13.4
DM1	10^{-3}	7.5
DMVISC	0.01	12.8
DPSILD	1.25	13.6
DPSILG	10.	13.6
DPSILD	1.25	13.6
DPSILN	10.	13.6
FRLCOM	8.2E14	12.5
FRACTV	-1	12.8
FRCMAX	0.	7.4.2
FRCMIN	10^{12}	7.4.2
FRLMAX	0.	7.4.2
FRLMIN	10^{13}	7.4.2
HCMASS	0	7.2.2
HMIX0	-1.	7.2
IACC	7	7.4.8
IACD	4	7.4.8
IACDP	4	13.2
IACPP	7	13.2
IATREF	1	7.4.4
IBC	3	13.4
IBCHE	1	12.8
IBFINT	1	13.6
IBPOPE	1	7.4.1
ICHANG	0	7.6
ICHANM	1	7.5
ICHC	0	13.5
ICHCKP	0	13.8
ICHCOO	0	12.5
ICOLHN	1	12.3.1
ICMDRA	0	12.5
ICOMDE	1	12.5
ICOMGR	0	12.8
ICOMPT	0	7.4.1, 12.5
ICOMRT	0	12.5
ICOMST	1	12.5
CONRE	0	7.8
ICONV	0	7.8
ICOOLP	0	13.8
ICRSW	0	13.7
IDCONZ	31	12.6
IDEEPC	2	7.8
IDGREY	0	13.3
IDLST	5	7.4.5
IDLTE	1000	7.4.4
IDMFIX	1	7.5

IELCOR	100	13.2
IFALI	5	7.4.3
IFCHTR	0	12.3.2
IFCIA	0	12.2.3
IFDIEL	0	12.3.3
IFENTR	0	12.7
IFIMXO	0	7.4.7
IFLEV	0 for NLTE	13.5
	1 for LTE	13.5
IFMOFF	0	13.6
IFMOL	0	7.4.1
IFPOPR	4	13.2
IFPREC	1	13.2
IFPRAD	0	7.9
IFPRD	0	12.9.1
IFRALI	0	7.4.3
IFRAYL	0	12.2.1
IFRYB	0	7.4.1
IFTENE	0	12.7
IFZ0	-1 (9 for disks)	12.8
IH2	0	13.3
IH2P	0	13.3
IHECOR	0	13.2
IHESO6	0	13.2
IHM	0	13.3
IHYDPR	0	12.1.1
IIRWIN	0	12.7
ILASCT	0	13.4
ILDER	0	13.6
ILGDER	0	12.6
ILMCOR	1	13.4
ILPSCT	0	13.4
IMUCON	0	7.8
INDL	0	7.4.7
	3 with convection	7.4.7
INHE	1	7.4.7
INMP	0	7.4.7
INPC	3	7.4.7
	4 with convection	7.4.7
INRE	2	7.4.7
INSE	4	7.4.7
	5 with convection	7.4.7
INTRPL	0	7.6
IOPH2P	0	12.2.2
IOPHE1	0	12.2.2
IOPHE2	0	12.2.2

IOPHMI	0	12.2.2
IOFTAB	0	7.4.1
IOSCOR	0	13.2
IOVER	1	13.6
IPOPAC	0	13.8
IPRESS	0	7.8
IPRIND	0	13.8
IPRING	0	7.5
IPRINP	0	13.8
IPRINT	0	7.8
IPTURB	1	7.2
IQUASI	0	12.1.2
IRDER	3	13.6
IRSCT	0	12.2.1
IRSPLT	1	13.2
ISPLIN	0	7.4.3
ISPODF	0	7.4.1, 7.7
ITEK	4	7.4.8
ITEMP	0	13.2
ITGMAX	10	7.5
ITLAS	100	13.6
ITMCOR	0	12.6
IVISC	0	7.2.3
IWINBL	-1	12.9.2
IZSCAL	0	7.2
JALI	1	7.4.3
JIDS	0	7.7
KNISH	0	12.5
KSNG	7	7.4.8
MLTYPE	0	7.2
MODREF	1	13.5
s NCCOUP	0	12.5
NCFOR1	0	12.5
NCFOR2	1	12.5
NCFULL	1	12.5
NCITOT	1	12.5
NCONIT	10	7.5
ND	70	7.4.6
NDCGAP	2	7.8
NDGREY	0	13.3
NDRE	0	7.4.5
NELSC	0	13.4
NFTAIL	21	7.4.2
NITER	30	7.4.6
NITZER	3	7.4.4
NLAMBD	2 (1 for LTE)	7.4.6, 13.2

NLAMT	1	13.2
NMU	3	7.4.6
NNEWD	0	7.5
NQUALP	3	12.1.2
NQUBAL	0	12.1.2
NQUBET	0	12.1.2
NQUGAM	0	12.1.2
NRETC	0	7.4.5
NTRALI	3	13.4
NQUALP	3	12.1.2
NQUBET	0	12.1.2
ORELAX	1.	7.4.8
POPZER	10^{-20}	7.4.4
POPZR2	10^{-20}	13.5
RADSTR	0	7.2.2
RADZER	10^{-20}	7.4.3
REYNUM	0.	7.2.3
RSOURC	0.	7.3
SPRFAC	0.667	7.3
STRL1	0.001	7.7
STRL2	0.02	7.7
STRLX	10^{-10}	7.7
SWPFAC	0.1	13.7
SWPINC	1.	13.7
SWPLIM	0.001	13.7
TAUDIV	0.5	7.4.5
TAUFIR	10^{-7}	7.5
TAULAS	316.	7.5
TDISK	0	7.5
TQMPRF	0	12.1.2
TRAD	0.	7.3
TSURF	0.	13.3
VTB	0.	7.2
XGRAD	0.	7.9
XPDIV	0	12.9.1
WDIL	1.	7.3
ZETA0	0.	7.2.3, 12.8
ZETA1	0.	7.2.3, 12.8

17 Outlook

TLUSTY has been under a continuous development for over three decades, and there is no reason to stop it now. We plan to do various upgrades on different levels to make the code even more flexible, efficient, and possibly also more

user-friendly.

We will first describe the upgrades or additions as far as the physical processes are concerned, going roughly from low temperatures to high.

- Including opacity and scattering due to condensates (clouds; dust). Since these are included in a special variant CoolTLUSTY, this upgrade is quite straightforward and needs only transporting the corresponding routines. The necessary tables were already constructed by Budaj et al. (2014) and made publicly available.

- Considering departures from chemical equilibrium for carbon and nitrogen chemistry, following the approach described in Hubeny & Burrows (2007). It is also implemented in CoolTLUSTY, so transporting the corresponding routines is straightforward.

- Developing additional and more sophisticated approaches for treating convection. Some are already included in CoolTLUSTY, but more are needed to cope with convergence and stability problems in some cases.

- There are several new promising approaches to treat convection beyond the framework of the mixing-length theory. We will explore them, and possibly implement and test them in TLUSTY.

- The treatment of occupation probabilities will be extended to treat also neutral perturbers.

- There is a theoretical development in progress (Gomez, in prep.) to replace the present treatment of pseudocontiua with a better and physically more realistic approach. That would provide a significant improvement in the accuracy of white dwarfs models.

On the high-energy side:

- Implementing a better treatment of inner-shell transitions.

- Implementing a treatment of K lines

- Upgrading the treatment of the Compton scattering to a fully relativistic case with Klein-Nishina cross section and the actual redistribution function to go beyond the Kompaneets approximation.

On an algorithmic level, we envisage several upgrades to help the efficiency and stability of the model construction. These include

- Modifying the Rybicki scheme to linearize with respect to T and N, not just T as it is at present.

- To extend the current rudimentary treatment of the over-relaxation acceleration to a more sophisticated approach.

- To provide an improved flexibility in treating partial opacity tables in a hybrid approach so that some species are treated as explicit and some through the opacity tables.

As to the global geometrical framework is concerned, we do not plan to further upgrade the current TLUSTY to treat 3-D effects and/or dynamical structures, because it requires a completely different philosophy of modeling. However, we plan to upgrade our 3-D radiation transfer solver program called IRIS (Ibgui et al. 2013) by transporting all routines from TLUSTY that describe local physics; in particular the evaluation of opacities, and the solution of the kinetic equilibrium equation with ALI and preconditioning, which would provide a means to construct NLTE models for snapshots of independent hydrodynamical calculations, and improved estimate of radiation moments to better describe the radiation energy density, flux, and pressure in hydrodynamical calculations.

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List of acronyms

We tried to keep the number of used acronyms at a minimum because a heavy usage of them is often annoying for a reader. We only used common acronyms, which we list below.

ALI	Accelerated Lambda Iteration
CFR	Complete Frequency Redistribution
CIA	Collision-Induced Absorption
CL	Complete Linearization
DFE	Discontinuous Finite Element (method)
LTE	Local Thermodynamic Equilibrium
ML2	modified Mixing Length prescription for convective flux
NLTE	non-LTE (any departure from LTE)
ODF	Opacity Distribution Function
OP	Opacity Project
OS	Opacity Sampling
PFR	Partial Frequency Redistribution
RAP	Resonance-Averaged Profile
SOR	Successive Over-Relaxation

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